Towards the quasi-localization of canonical GR*

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Abstract

A general framework for a systematic quasi-localization of canonical general relativity and a new ingredient, the requirement of the gauge invariance of the boundary terms appearing in the calculation of Poisson brackets, are given. As a consequence of this it is shown, in particular, that the generator vector fields (built from the lapse and shift) of the quasi-local quantities must be divergence free with respect to a Sen-type connection; and the volume form induced from the spatial metric on the boundary surface must be fixed.

1 Introduction

Conserved quantities have always had distinguished role in physics. Though for a general system no systematic way of finding them is known, but for systems whose dynamics can be described by a Hamiltonian in the canonical framework there is a way. The first systematic investigation of Einstein's general relativity (GR) in its canonical form was done in the ADM variables and was focused on asymptotically flat configurations [1]. One of the key objects in the canonical formulation of the vacuum general relativity is the constraint function ('parameterized' by a function N and a vector field N^a on the manifold Σ, called the lapse and the shift, respectively):

$$C\big[N,N^e\big]:=-\int_\Sigma\Big\{\frac{1}{2\kappa}\Big(R-2\lambda+\frac{4\kappa^2}{|h|}\big[\frac{1}{n-1}\tilde p^2-\tilde p_{ab}\tilde p^{ab}\big]\Big)N\sqrt{|h|}+ \\ +\big(2D_a\tilde p^{ab}\big)h_{bc}N^c\Big\}\mathrm{d}^nx. \tag{1.1}$$

Here the canonical variables are the fields h_{ab} and $\tilde p^{ab}$ on the connected n-manifold Σ, h_{ab} being the (negative definite) spatial metric, D_e is the corresponding Levi-Civita covariant derivative, R is its curvature scalar and $\kappa:=8\pi G$ with Newton's gravitational constant G, and we allow a nontrivial cosmological constant λ to be present. (Though primarily we are interested in the physical (3+1) dimensional case, the analysis can be done in $(n+1)$ dimensions without any extra effort, but $n\geq 2$.)

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One of the basic observations of Arnowitt, Deser and Misner is that the constraint functions play a double role in the dynamics of GR (see also [2]). In fact, the *constraint* part of Einstein's equations is equivalent to $C[N, N^e] = 0$ for every N and N^e and their *formal* variational derivatives with respect to the canonical variables (given explicitly by (2.2)-(2.3)) appear in the canonical equations of motion, which are just the *evolution parts* of the field equations:

$$\dot{h}_{ab} = \frac{\delta H\big[N, N^e\big]}{\delta \tilde{p}^{ab}}, \qquad \dot{\tilde{p}}^{ab} = -\frac{\delta H\big[N, N^e\big]}{\delta h_{ab}}, \tag{1.2}$$

where now $H[N, N^e] = C[N, N^e]$. Thus, apparently, it is the constraints that generate the evolution of the states of the theory through the canonical equations of motion in the phase space, i.e. the constraint functions appear to play the role of the Hamiltonian in the canonical formulation of general relativity. Another important observation of Arnowitt, Deser and Misner is that by the integral of the Landau–Lifshitz pseudotensor in an asymptotically Cartesian coordinate system, the total energy and linear momentum can be introduced, and these quantities turned out to be conserved during the time evolution of the system.

However, as Regge and Teitelboim pointed out [3], the constraint functions $C[N, N^e]$ with the $1/r$ and $1/r^2$ fall-off for the canonical variables are *not* functionally differentiable in the strict sense (see e.g. [4]). The total variation of $C[N, N^e]$ with respect to h_{ab} and $\tilde{p}^{ab}$ yields not only the expected volume terms, i.e. the *formal* variational derivatives (2.2)-(2.3) contracted with δh_{ab} and $\delta\tilde{p}^{ab}$, respectively, but integrals on the boundary of Σ at infinity as well (see equation (2.1)). Thus, strictly speaking, the functional derivatives of $C[N, N^e]$ are the sums of smooth fields and *distributions* concentrated on the boundary of Σ. Therefore, if we want to recover the correct evolution equation for the smooth tensor fields as the Hamiltonian equations of motion (rather than some distributional generalization of them), then the Hamiltonian must be functionally differentiable with respect to the canonical variables. Since adding a boundary integral to $C[N, N^e]$ does not change the formal functional derivatives, Regge and Teitelboim searched for the correct Hamiltonian in the form

$$H\big[N, N^e\big] = C\big[N, N^e\big] + \frac{1}{\kappa}\oint_{\mathcal{S}} B\big(N, N^e\big)\mathrm{d}\mathcal{S}, \tag{1.3}$$

where the integral on $\mathcal{S}$ is understood as the $r \to \infty$ limit of the integrals on large spheres of radius r in the asymptotically flat ends of Σ and $B(N, N^e)$ is some expression of the canonical variables and a *linear* expression of N and N^e. They showed that there is, indeed, a boundary term which makes (1.3) differentiable. Moreover, as a bonus, for appropriately chosen (N, N^e) this Hamiltonian automatically reproduces the total energy and linear momentum of Arnowitt, Deser and Misner as its value on the constraint surface and, in addition, the spatial angular momentum and centre-of-mass could also be introduced. Thus, the claim of a pure mathematical consistency yielded a physically highly desirable result.

Nevertheless, as Beig and Ó Murchadha [5] showed, the asymptotic form of N and N^e should not be prescribed by hand. That is a consequence of the requirement of the compatibility of the boundary conditions and the evolution equations: Since the evolution equations involve the lapse and the shift, and they must preserve the boundary conditions imposed on the canonical variables, we get a restriction on the asymptotic form of N and N^e. In fact, in the leading order they depend on the asymptotically Cartesian *spatial*

coordinates just like the Killing vectors of Minkowski spacetime. (On the other hand, the time dependence of N and N^e remained unrestricted.) Without this compatibility condition the initial data set, satisfying the boundary conditions at the initial instant, would evolve in the next instant into a new data set that would *not* belong to the actual phase space, i.e. the evolution would take a data set out of the phase space. Beig and Ó Murchadha refined the Hamiltonian of Regge and Teitelboim, too, such that the new Hamiltonian is not only functionally differentiable, but finite on the whole phase space (rather than only on the constraint surface), and that these Hamiltonians form a Lie algebra with respect to the Poisson bracket as the Lie product. The constraints form a Lie ideal in this algebra, and their quotient, the algebra of observables, is isomorphic to the Poincaré algebra. The conserved quantities then become coordinates in this quotient algebra.

Since the evolution equations specify only how the lapse and the shift depend asymptotically on the *spatial* coordinates but not on the time coordinate, moreover the spatial angular momentum and the centre-of-mass of Beig and Ó Murchadha do not transform in the correct way under an asymptotic Poincaré transformation *in the spacetime*, further refinements of the previous results were needed. As a resolution of these difficulties in [6, 7] a distinction between the evolution vector fields that should be used in the Hamiltonian to generate the evolution of the states and the vector fields built from the lapse and the shift that should be used to define ADM type conserved quantities was made. The latter must be the asymptotic spacetime Killing fields, which turned out to be a special case of the former.

In the present paper, these ideas will be applied to the case in which the manifold Σ is compact with a smooth boundary $\mathcal{S} := \partial\Sigma$, i.e. at the quasi-local level (see e.g. [8]). Thus, now we are interested in the Hamiltonian dynamics of general subsystems of the universe. The extension of the investigations of canonical general relativity to the quasi-local case is required by solving several problems. First, to have a deeper understanding of the (geometrical or thermodynamical) properties of black holes, for example to formulate the various (geometric) inequalities or the entropy bounds for black holes, the conserved quantities or, more generally, the observables of the gravitational 'field' must be introduced quasi-locally. A further motivation of searching for quasi-local observables is the remarkable result of Torre [9] that all the global observables for the vacuum gravitational field in a closed universe, built as spatial integrals of local functions of the initial data and their finitely many derivatives, are necessarily vanishing. Thus in closed universes we can associate non-trivial, locally constructible observables only with subsystems, bounded at one instant by some closed spacelike 2-surface. Another motivation is the claim to see the content of the basic existence and uniqueness results of Friedrich and Nagy [10] for the initial-boundary value problem for the vacuum Einstein equations from the Hamiltonian point of view.

Though the first few steps towards the systematic quasi-localization of canonical general relativity using the ADM variables have already been done [11], the project remained incomplete and essential new ideas were needed. In the present paper, we continue these investigations. We refine our previous framework, and, in addition to the ideas introduced in the asymptotically flat context (and discussed above), only first principles (such as gauge invariance in every sense, covariance, etc), but no ad hoc ideas or elements (e.g. some a priori reference configuration, gauge choice or even implicitly given background structure) will be used. We think that these would contradict the principle of equivalence (see also [12]) and hence the very spirit of Einstein's general relativity. It is the theory

itself that should tell us what the boundary conditions, the observables, etc are, and we must read off these from the structure of the theory itself. For a different view (but an absolutely legitimate strategy), see e.g. [13].

Though in the present paper we cannot complete the quasi-localization programme, we raise a new issue that should be discussed in connection with the quasi-localization of canonical GR. Namely, we argue that the boundary terms appearing in the calculation of the Poisson bracket of two Hamiltonians must be gauge invariant in every sense. We show that the requirement of this gauge invariance yields a restriction on the lapse and shift: the generator vector field built from them according to $K^a = Nt^a + N^a$, where t^a is the future pointing unit timelike normal to the spacelike hypersurfaces Σ in the spacetime, must be divergence free with respect to the Sen-type connection induced on the boundary, $\Delta_a K^a = 0$. Remarkably enough, this is one of the ten (or, in $(n+1)$ dimensions, the $\frac{1}{2}(n+1)(n+2)$) spacetime Killing equations. A consequence of this condition is that the induced volume form $\varepsilon_{e_1 \dots e_{n-1}}$ on the boundary $\mathcal{S}$ remains constant during the evolution, and hence it is natural to impose $\delta\varepsilon_{e_1 \dots e_{n-1}} = 0$. $\delta\varepsilon_{e_1 \dots e_{n-1}} = 0$, as a part of the boundary conditions for the canonical variables, has already been found in special contexts, e.g. in connection with the functional differentiability of the constraint functions. The present investigations show that $\delta\varepsilon_{e_1 \dots e_{n-1}} = 0$ should be a part of the 'ultimate' boundary conditions, too.

In the following section we formulate (and refine the previous attempts of) the quasi-localization programme of canonical GR and discuss the tools and the technical details that we need as well as the partial results. In section 3 we quasi-localize the canonical formulation of a single, real scalar field, and we will see that the boundary terms appearing in the Poisson bracket of two Hamiltonians should be interpreted as the energy-momentum and angular momentum flux, and hence a gauge invariant observable. In subsection 4.1, we return to general relativity and study the analogous boundary terms in the Poisson bracket of two constraints. We derive here the boundary conditions $\Delta_a K^a = 0$ and $\delta\varepsilon_{e_1 \dots e_{n-1}} = 0$. Finally, in subsection 4.2, we find arguments both in favour of and against a Hamiltonian boundary term which is the basis of several suggestions for the quasi-local energy-momentum. Though there are a number of key issues even in connection with the present partial results (e.g. how they are related to the maximal dissipative boundary condition of Friedrich and Nagy [10]), we should leave these to a future investigation.

Our notations and conventions are essentially those that were used in [11]. In particular, we use the abstract index formalism, the signature of the spacetime metric is $1-n$, and the curvature is defined by $-R^a{}_{bcd}X^b := (D_c D_d - D_d D_c)X^a$. The analysis is based on certain formulae given explicitly in [6, 11]. Our standard reference in canonical formalism is [14].

2 The quasi-localization programme

2.1 The general programme

2.1.1 The basic requirements

In the quasi-local canonical formulation of general relativity, the basic object is the quasi-local configuration space $\mathcal{Q}(\Sigma)$ over the connected n-manifold Σ with smooth boundary $\mathcal{S} := \partial\Sigma$. This is the space of smooth (negative definite) metrics h_{ab} on Σ satisfying certain not-yet-specified boundary conditions on $\mathcal{S}$. The quasi-local phase space is defined to be

its 'cotangent bundle' $T^*\mathcal{Q}(\Sigma)$, endowed with the natural symplectic structure. Thus the elements of the quasi-local phase space are the pairs $(h_{ab}, \tilde{p}^{ab})$ of fields, where $\tilde{p}^{ab}$ is a symmetric contravariant tensor density of weight one. ($\tilde{p}^{ab}$ is usually interpreted as a 1-form at the point $h_{ab} \in \mathcal{Q}(\Sigma)$: if $h_{ab}(u)$ is any smooth 1-parameter family of metrics such that $h_{ab}(0) = h_{ab}$, i.e. $h_{ab}(u)$ is a 'curve' in $\mathcal{Q}(\Sigma)$ through h_{ab}, then the tensor field δh_{ab} on Σ, defined pointwise as $\delta h_{ab}(p) := (\mathrm{d}h_{ab}(p,u)/\mathrm{d}u)|_{u=0}$, $\forall p \in \Sigma$, is called the tangent of the 'curve' at h_{ab}. In fact, the directional derivative of any functionally differentiable function $F : \mathcal{Q}(\Sigma) \to \mathbb{R}$ along the 'curve' at the point h_{ab} is $\delta F := (\mathrm{d}F(h_{ab}(u))/\mathrm{d}u)|_{u=0} = \int_\Sigma \frac{\delta F}{\delta h_{ab}} \delta h_{ab} \mathrm{d}^n x$, which defines the action of δh_{ab} on any such F and the natural pairing of δh_{ab} and the 'exact 1-form' $dF = \frac{\delta F}{\delta h_{ab}}$ at the same time. Thus, it is natural to define the action of $\tilde{p}^{ab}$ on the 'tangent vector' δh_{ab} at the point $h_{ab} \in \mathcal{Q}(\Sigma)$ by the integral $\int_\Sigma \delta h_{ab} \tilde{p}^{ab} \mathrm{d}^n x$. Note that while in the asymptotically flat context the requirement of the finiteness of the integral $\int_\Sigma \delta h_{ab} \tilde{p}^{ab} \mathrm{d}^n x$ together with the evolution equations restrict the fall-off rate k of the metric, namely [6] it must be $k \geq \frac{1}{2}(n-1)$, in the quasi-local case we obtain no restriction for the canonical variables.) Clearly, the differentiability of functions on the quasi-local phase space depends not only on the function itself, but on the boundary conditions that are imposed on the canonical variables in the definition of $T^*\mathcal{Q}(\Sigma)$. We stress that the boundary conditions are parts of the definition of the phase space. (For a more detailed discussion of this issue, see e.g. [15].) The canonical symplectic structure can be characterized equivalently by specifying the Poisson bracket of any two *functionally differentiable* functions. For any such G and $H : T^*\mathcal{Q}(\Sigma) \to \mathbb{R}$, it is $\{G, H\} := \int_\Sigma (\frac{\delta G}{\delta \tilde{p}^{ab}} \frac{\delta H}{\delta h_{ab}} - \frac{\delta H}{\delta \tilde{p}^{ab}} \frac{\delta G}{\delta h_{ab}}) \mathrm{d}^n x$.

In a more pedagogical approach the lapse and the shift are also considered to be configuration variables (see e.g. [16]), and there are additional constraints (the 'primary constraints') that the momenta conjugate to the lapse and the shift are vanishing. Then a systematic constraint analysis shows that this 'big' phase space $T^*\tilde{\mathcal{Q}}(\Sigma)$ can always be reduced to $T^*\mathcal{Q}(\Sigma)$ in a straightforward way, and the role of the lapse and the shift is reduced from dynamical variables only to 'parameters'. In this sense, $T^*\mathcal{Q}(\Sigma)$ can also be considered as a 'partially reduced' phase space. We save this reduction by starting with $T^*\mathcal{Q}(\Sigma)$ as the phase space.

Our ultimate aim is the quasi-localization of canonical general relativity, i.e. finding

1. a boundary term $B(N, N^e)$ (we will call its integral the Hamiltonian boundary term), built from the canonical variables and depending linearly on the lapse and the shift;
2. boundary conditions for the canonical variables $(h_{ab}, \tilde{p}^{ab})$ on $\mathcal{S}$;
3. boundary conditions for the lapse N and the shift N^e on $\mathcal{S}$

such that

i. the Hamiltonian $H : T^*\mathcal{Q}(\Sigma) \to \mathbb{R}$, given by (1.3) and 'parameterized' by lapses and shifts satisfying the boundary conditions in point 3, is functionally differentiable with respect to the canonical variables;

ii. the evolution equations (1.2) with lapses and shifts satisfying the boundary condition in point 3. above preserve the boundary conditions imposed on the canonical variables in point 2;

iii. the constraints close to a Poisson algebra $\mathcal{C}$ (which we call the quasi-local constraint algebra);

iv. the value of the Hamiltonian on the constraint surface (i.e. if $C[N, N^e] = 0$) must be a $2 + (n-1)$-covariant, gauge-invariant expression of the boundary data on $\mathcal{S}$.

Before turning to the mathematical realization of these requirements we should discuss these points.

2.1.2 The discussion of the requirements

Clearly, requirement (i) is just that of Regge and Teitelboim [3], and (ii) is taken from Beig and Ó Murchadha [5]. While the first is a generally accepted condition in the relativity community, the second is apparently not appreciated enough. Moreover, the usual (and in the quasi-local canonical approaches almost exclusively adopted) view is that the lapse and the shift on the boundary $\mathcal{S}$ should be arbitrary, just because they are thought of as the $n+1$ pieces of the spacetime evolution vector field, and their arbitrariness are thought to express our freedom to choose the fleet of observers in the spacetime as we wish.

However, as we learnt from the structure of canonical GR of asymptotically flat spacetimes, requirement (ii) may yield non-trivial restrictions on the lapse and the shift. Moreover, as the study of the quasi-local conserved quantities of matter fields in Minkowski spacetime shows (and as we summarize the basic things in subsection 3.1), we must make a distinction between the *symmetries* (which define the conserved quantities) and the general *evolution vector fields* (which are used to define the time evolution of the initial data set in the spacetime). The former is the solutions of a linear partial differential equation (and the number of their independent solutions is finite), but the latter is quite arbitrary. Thus, in general relativity, the lapse and shift parts of a general evolution vector field may be, but the lapse and shift parts of a vector field defining 'conserved' quantities are probably restricted. In particular, as we will see in subsection 2.3.3, the 'most natural' quasi-local Hamiltonian cannot provide an acceptable expression for the energy-momentum if the lapse and shift on $\mathcal{S}$ are chosen independently of the canonical variables. We expect that these conditions are given only implicitly, possibly in the form of a system of *linear* partial differential equations (p.d.e.) on $\mathcal{S}$. In fact, in section 4 we derive an equation for the lapse and shift which should be a part of such a system of linear p.d.e.

Requirement (iii) expresses the claim that the gauge content of the theory must be represented in a correct way by the constraints even quasi-locally. The motivation of this expectation comes from the applicability of the standard canonical formalism (see e.g. [14]). In fact, for $n \geq 3$ general relativity is expected to have internal degrees of freedom, which are expected to be represented in the canonical framework by the points of the reduced phase space. However, strictly speaking the reduced phase space can be formed as the space of gauge orbits in the constraint surface only when the Hamiltonian vector fields of the constraint functions form an involutive distribution or, equivalently, if the constraint functions close to a Poisson algebra.

Though in the asymptotically flat case the Hamiltonians of Beig and Ó Murchadha also close to a Poisson algebra (in which the constraints form an ideal) [5], we will see in subsection 3.2.2 that quasi-locally this is not true even for the scalar field, and hence

it cannot be expected in general relativity either. In fact, the boundary terms appearing in the Poisson bracket of two Hamiltonians (and which destroy the Poisson algebra structure) describe incoming and outgoing energy-momentum and angular momentum fluxes. Thus quasi-locally the algebra of observables is much bigger than the set of the Hamiltonians.

In the present investigations, we do not use any 'natural' (or rather ad hoc) conditions e.g. for the canonical variables. We use only first principles, such as gauge invariance (in any sense) or covariance. Requirement (iv) is the manifestation of this idea. In particular, the boundary term $B(N, N^e)$ should not depend on the normal directional derivatives of the lapse and the shift, or on the actual lapse and shift separately, but only on their spacetime-covariant combination $K^e := Nt^e + N^e$. Moreover, it should not depend on the actual choice for the normals (t^a, v^a) of $\mathcal{S}$ but only on the intrinsic and extrinsic *geometry* of $\mathcal{S}$ (but not e.g. on the extension of the geometrical quantities off $\mathcal{S}$).

However, because of the strong interplay between the Hamiltonian boundary term and the boundary conditions both for the canonical variables and the lapse and shift, it would be extremely difficult to determine these *three* unknown things in a single step. Indeed, in the traditional approach usually one of these three is a priori given, and by the requirements (i) and (ii) we can determine the other two in a relatively straightforward way. For example, in the asymptotically flat case we have a priori boundary conditions, from which Beig and Ó Murchadha could determine both the Hamiltonian boundary term and the boundary conditions for the lapse and shift. In subsection 2.3 we summarize the special cases in which various Hamiltonian boundary terms were a priori given, from which the boundary conditions could be determined. (The necessary tools and technical ingredients will be summarized in subsection 2.2.) Thus, in order to be able to manage the general problem, a new idea would be needed.

As we already mentioned in the introduction, such a new idea could be the observation that the boundary terms in the Poisson bracket of two Hamiltonians (which we call the Poisson boundary term) should be the sum of the Hamiltonian boundary term and terms analogous to the energy-momentum and angular momentum flows between the system and the rest of the universe, and hence these must be gauge invariant. This idea is based on the moral of the analogous investigations of a scalar field, the subject of section 3.

2.2 The main ingredients

2.2.1 The variational formula

Though formally the manifold Σ on which the canonical variables $(h_{ab}, \tilde{p}^{ab})$ as fields are defined is an abstract n-manifold, it is convenient (and illuminating, and hence useful) to consider this as the typical leaf of a foliation $\{\Sigma_t\}$ of (a piece of) the spacetime by spacelike hypersurfaces and identify Σ at the coordinate time instant t with Σ_t. Thus although in the phase-space context there is no reason to speak about the normal of Σ, in the spacetime we have a uniquely defined future pointing unit timelike normal t^a of the leaves Σ_t (and hence a projection $P^a_b := \delta^a_b - t^a t_b$ of the spacetime tangent spaces to the tangent spaces of the leaves, too), and we frequently rewrite formulae given in the phase-space context to its spacetime form or vice versa freely if needed. For example, the spacetime form of the lapse and the shift is the so-called evolution vector field $\xi^a = Nt^a + N^a$, by means of which the spacetime form of the constraint function (1.1) is just the integral $C[\xi^e] := \frac{1}{\kappa}\int_\Sigma \xi^a({}^M G_{ab} + \lambda g_{ab})t^b \mathrm{d}\Sigma$. Here g_{ab} is the spacetime metric, ${}^M G_{ab}$ is the corresponding Einstein tensor and the induced volume element on Σ

is $\mathrm{d}\Sigma := \frac{1}{n!}t^e\varepsilon_{ea_1\dots a_n}$. ($\varepsilon_{a_1\dots a_{n+1}}$ is the volume $(n+1)$-form in the spacetime.) Note that the timelike unit normal to Σ is globally well defined if the spacetime is time orientable.

Also, we will need the expression of the canonical momentum in terms of the Lagrange variables, i.e. the configuration and velocity variables. The latter is defined with respect to some spacetime vector field ξ^e such that the hypersurfaces Σ_t of the foliation are obtained from Σ by Lie dragging along the integral curves of ξ^e. We assume that these hypersurfaces are spacelike. Let t^a be their future pointing unit timelike normal, the lapse and the shift parts of ξ^e are $N := t_e\xi^e$ and $N^e := P^e_f\xi^f$, respectively, and the acceleration of the hypersurfaces is $a_e := t^a\nabla_a t_e = -D_e \ln N$. Here D_e denotes the induced Levi-Civita derivative operator on $T\Sigma_t$. The time derivative of a purely *spatial* tensor field $T^{a\dots}_{b\dots}$ is defined to be the projection to the hypersurfaces of its Lie derivative along ξ^e, i.e. $\dot{T}^{a\dots}_{b\dots} := (L_\xi T^{c\dots}_{d\dots})P^a_c\dots P^d_b\dots = N(L_{\mathbf{t}}T^{c\dots}_{d\dots})P^a_c\dots P^d_b\dots + L_{\mathbf{N}}T^{a\dots}_{b\dots}$. In particular, $\dot{h}_{ab} = 2N\chi_{ab} + L_{\mathbf{N}}h_{ab}$. Thus essentially the extrinsic curvature χ_{ab} of the leaves of the foliation plays the role of the velocity, by means of which the canonical momentum is known to be $\tilde{p}^{ab} = \frac{1}{2\kappa}\sqrt{|h|}(\chi^{ab} - \chi h^{ab})$. Here χ is the h_{ab}-trace of χ_{ab}.

To calculate the total variation of (1.1), let $N(u)$, $N^a(u)$, $h_{ab}(u)$ and $\tilde{p}^{ab}(u)$, $u \in (-\epsilon, \epsilon)$, be any smooth 1-parameter families of lapses, shifts, metrics and canonical momenta, respectively. Then we define the corresponding variation of any of their function, $F = F(N, N^a, h_{ab}, \tilde{p}^{ab})$, to be its u-derivative at $u = 0$, i.e. $\delta F := (\mathrm{d}F(N(u), N^a(u), h_{ab}(u), \tilde{p}^{ab}(u))/\mathrm{d}u)|_{u=0}$. The corresponding variation of the constraint function $C[N, N^e]$, taken from [6], is

$$\begin{aligned}\delta C\bigl[N,N^e\bigr] = &C\bigl[\delta N,\delta N^e\bigr] + \int_\Sigma\Bigl(\frac{\delta C[N,N^e]}{\delta h_{ab}}\delta h_{ab} + \frac{\delta C[N,N^e]}{\delta\tilde{p}^{ab}}\delta\tilde{p}^{ab}\Bigr)\mathrm{d}^n x +\\ &+\frac{1}{2\kappa}\oint_{\partial\Sigma}\Bigl\{\, N\bigl(h^{ab}v^e(D_e\delta h_{ab}) - v^a(D^b\delta h_{ab})\bigr) + \bigl(v^aD^bN - h^{ab}v^eD_eN\bigr)\delta h_{ab}\\ &\qquad + \frac{2\kappa}{\sqrt{|h|}}\bigl(2N^a v_e\tilde{p}^{eb} - N^e v_e\tilde{p}^{ab}\bigr)\delta h_{ab} + 4\kappa N_a v_b\frac{\delta\tilde{p}^{ab}}{\sqrt{|h|}}\Bigr\}\mathrm{d}\mathcal{S}. \qquad (2.1)\end{aligned}$$

Here v^a is the *outward* pointing unit normal of $\mathcal{S}$ in Σ, $\mathrm{d}\mathcal{S}$ is the induced volume element on the boundary, and the *formal* variational derivatives are

$$\begin{aligned}\frac{\delta C[N,N^e]}{\delta h_{ab}} := &\frac{1}{2\kappa}\sqrt{|h|}\Bigl\{N\Bigl(R^{ab} - Rh^{ab} + 2\lambda h^{ab} + \frac{8\kappa^2}{|h|}\bigl(\tilde{p}^a{}_c\tilde{p}^{cb} -\\ &-\frac{1}{n-1}h_{cd}\tilde{p}^{cd}\tilde{p}^{ab}\bigr)\Bigr) + D^aD^bN - h^{ab}D_cD^cN\Bigr\} - L_{\mathbf{N}}\tilde{p}^{ab} +\\ &+\frac{1}{4\kappa}Nh^{ab}\sqrt{|h|}\Bigl(R - 2\lambda + \frac{4\kappa^2}{|h|}\bigl(\frac{1}{n-1}\tilde{p}^2 - \tilde{p}^{cd}\tilde{p}_{cd}\bigr)\Bigr), \qquad (2.2)\\ \frac{\delta C[N,N^e]}{\delta\tilde{p}^{ab}} := &\frac{4\kappa}{\sqrt{|h|}}N\Bigl(\tilde{p}_{ab} - \frac{1}{n-1}\tilde{p}^{cd}h_{cd}h_{ab}\Bigr) + L_{\mathbf{N}}h_{ab}. \qquad (2.3)\end{aligned}$$

Here R_{ab} is the Ricci tensor of D_e, and note that the last line of (2.2) is $-\frac{1}{2}h^{ab}$ times the integrand of the constraint function $C[N,0]$.

Therefore, $C[N,N^e]$ is functionally differentiable (in the strict sense of [4]) with respect to the canonical variables only if the boundary integral in (2.1) is vanishing, in which case the functional derivatives themselves are given by (2.2) and (2.3). Then, provided the constraints are satisfied, the vacuum evolution equations (with the cosmological constant) are precisely the canonical equations of motion (1.2).

2.2.2 A quick review of the geometry of the boundary surface

To evaluate the boundary terms in (2.1), it seems useful to split the variation of the metric h_{ab} at the points of $\mathcal{S}$ with respect to the boundary. Moreover, in the subsequent subsections several expressions on $\mathcal{S}$, obtained originally in the traditional $n+1$ form, will have to be rewritten in a $2+(n-1)$ form. Nevertheless, most of these notions have a non-trivial meaning only if $n \geq 3$; and hence when we use them we assume that $n \geq 3$. Thus now, in a nutshell, we summarize the basic geometric objects that we need in what follows. A more detailed discussion of these concepts is given e.g. in [17, 8].

To avid confusion, the Kronecker delta on Σ will be denoted by P^a_b, and the h_{ab}-orthogonal projection to $\mathcal{S}$ is $\Pi^a_b := P^a_b + v^a v_b$. Then the induced metric and the corresponding intrinsic Levi-Civita covariant derivative on $\mathcal{S}$ is $q_{ab} := h_{cd}\Pi^c_a\Pi^d_b$ and $\bar\delta_e$, respectively, and let us introduce another derivative operator simply by $\bar\Delta_e := \Pi^f_e D_f$. The extrinsic curvature of $\mathcal{S}$ in Σ will be defined by $\nu_{ab} := \Pi^c_a\Pi^d_b D_c v_d$. The difference of these two derivative operators is just the extrinsic curvature: $\bar\Delta_e X^a = \bar\delta_e(\Pi^a_b X^b) - v^a\bar\delta_e(v_b X^b) + (\nu_{eb}v^a - \nu_e{}^a v_b)X^b$ for any X^a tangent to Σ. The induced volume $(n-1)$ form and volume element on $\mathcal{S}$ are $\varepsilon_{e_1\dots e_{n-1}} := t^a v^b \varepsilon_{abe_1\dots e_{n-1}}$ and $\mathrm{d}\mathcal{S} := \frac{1}{(n-1)!}t^a v^b \varepsilon_{abe_1\dots e_{n-1}}$, respectively. Note that with these conventions, the Gauss theorem takes the form $\int_\Sigma D_a X^a \mathrm{d}\Sigma = -\oint_{\mathcal{S}} v_a X^a \mathrm{d}\mathcal{S}$ for any vector field X^a on Σ.

The boundary $\mathcal{S} = \partial\Sigma$ can be considered as a submanifold in the spacetime, too. In the spacetime context the induced metric is $q_{ab} = g_{cd}\Pi^c_a\Pi^d_b$, and the area 2-form on the 2-planes normal to $\mathcal{S}$ is ${}^\perp\varepsilon_{ab} := t_a v_b - t_b v_a$. Here, both the projection Π^a_b and the area 2-form ${}^\perp\varepsilon_{ab}$ are independent of the actual choice of the normals (t^a, v^a). Note that the normals are not specified by $\mathcal{S}$, but if $\mathcal{S}$ is considered to be the boundary of Σ, then they are chosen as in the previous paragraph. If $\mathcal{S}$ is orientable and at least a neighbourhood of $\mathcal{S}$ in M is space and time orientable, then (t^a, v^a) can be chosen to be globally defined, yielding a global trivialization of the normal bundle $N\mathcal{S}$ of $\mathcal{S}$ in M. The two derivative operators Δ_e and δ_e, acting on any Lorentzian $n+1$ vector field X^a, are defined by $\Delta_e X^a := \Pi^f_e \nabla_f X^a$ and $\delta_e X^a := \Pi^a_b \Delta_e(\Pi^b_c X^c) + (\delta^a_b - \Pi^a_b)\Delta_e((\delta^b_c - \Pi^b_c)X^c)$. The extrinsic curvature tensor of $\mathcal{S}$ in M is $Q^a{}_{eb} := -\Pi^a_c \Delta_e \Pi^c_b = \tau^a{}_e t_b - \nu^a{}_e v_b$, where τ_{ab} and ν_{ab} are the individual (symmetric) extrinsic curvatures of $\mathcal{S}$ in M corresponding to the unit normals t_a and v_a, respectively. The corresponding traces are $\tau := \tau_{ab}q^{ab}$ and $\nu := \nu_{ab}q^{ab}$, respectively. The difference of the two derivative operators is this extrinsic curvature tensor: $\Delta_e X^a = \delta_e X^a + (Q^a{}_{eb} - Q_{be}{}^a)X^b$. δ_e is not only the Levi-Civita derivative operator $\bar\delta_e$ on the tangent bundle of $\mathcal{S}$, but it acts on the normal bundle $N\mathcal{S}$ of $\mathcal{S}$, spanned by the two normals t^a and v^a, as well. Its action can be characterized by the connection 1-form $A_e := (\Delta_e t_a)v^a = (\delta_e t_a)v^a$. On the other hand, for vectors tangent to Σ in M the two derivative operators $\bar\Delta_e$ and Δ_e coincide, which fact will be used several times when we rewrite expressions given in the $n+1$ form into its $2+(n-1)$ form.

At the points of $\mathcal{S}$, the splitting $h_{ab} = q_{ab} - v_a v_b$ implies the variation $\delta h_{ab} = \delta q_{ab} - v_a \delta v_b - v_b \delta v_a$. It is straightforward to determine the various projections of δh_{ab} (for details see [11]). These are

$$
\begin{aligned}
&\delta h_{cd}\Pi^c_a\Pi^d_b = \delta q_{cd}\Pi^c_a\Pi^d_b, \qquad \delta h_{cd}v^c\Pi^d_b = -\delta v^a q_{ab},\\
&\delta h_{cd}v^c v^d = 2v^a\delta v_a = -2v_a\delta v^a.
\end{aligned}
\tag{2.4}
$$

Thus the independent variations can be represented by $\delta q_{cd}\Pi^c_a\Pi^d_b$ and δv^a.

The curvature of the connections δ_e and Δ_e, respectively, are given by

$$
\begin{aligned}
f^a{}_{bcd} &= -{}^\perp\varepsilon^a{}_b\big(\delta_c A_d - \delta_d A_c\big) + {}^{\mathcal{S}}R^a{}_{bcd}, && (2.5)\\
F^a{}_{bcd} &= f^a{}_{bcd} - \delta_c\big(Q^a{}_{db} - Q_{bd}{}^a\big) + \delta_d\big(Q^a{}_{cb} - Q_{bc}{}^a\big) + \\
&\quad + Q^a{}_{ce}Q_{bd}{}^e + Q_{ec}{}^a Q^e{}_{db} - Q^a{}_{de}Q_{bc}{}^e - Q_{ed}{}^a Q^e{}_{cb}, && (2.6)
\end{aligned}
$$

where ${}^{\mathcal{S}}R^a{}_{bcd}$ is the curvature tensor of the intrinsic Levi-Civita connection $\bar\delta_e$ of $(\mathcal{S}, q_{ab})$. Of course, for $n=3$, it can also be written in the form $\frac{1}{2}{}^{\mathcal{S}}R(\Pi^a_c q_{bd} - \Pi^a_d q_{bc})$, where ${}^{\mathcal{S}}R$ is the curvature scalar. The curvature $F^a{}_{bcd}$ turns out to be just the pull-back to $\mathcal{S}$ of the spacetime curvature 2-form: $F^a{}_{bcd} = {}^M R^a{}_{bef}\Pi^e_c\Pi^f_d$. Its various projections,

$$
\begin{aligned}
\Pi^e_a\Pi^f_b F_{efcd} &= {}^{\mathcal{S}}R_{abcd} + \tau_{ac}\tau_{bd} - \tau_{ad}\tau_{bc} - \nu_{ac}\nu_{bd} + \nu_{ad}\nu_{bc}, && (2.7)\\
t^a\Pi^f_b F_{afcd} &= \delta_c\tau_{db} - \delta_d\tau_{cb} + A_c\nu_{db} - A_d\nu_{cb}, && (2.8)\\
v^a\Pi^f_b F_{afcd} &= \delta_c\nu_{db} - \delta_d\nu_{cb} + A_c\tau_{db} - A_d\tau_{cb}, && (2.9)\\
t^a v^b F_{abcd} &= \tau_{ec}\nu^e{}_d - \tau_{ed}\nu^e{}_c + \delta_c A_d - \delta_d A_c, && (2.10)
\end{aligned}
$$

are the so-called Gauss, Codazzi–Mainardi, and Ricci equations.

2.3 Special cases

2.3.1 The quasi-local constraint algebra

A special, genuinely quasi-local case in which the programme could be completed is when there is no Hamiltonian boundary term, i.e. when we are interested in the boundary conditions both for the canonical variables and for the lapse and shift that make the *constraint* functions functionally differentiable and close to a Poisson algebra. The significance of this special case is that the constraints represent those parts of the field equations that are expected to generate the gauge motions in phase space. Thus to understand the gauge content of GR at the quasi-local level, we should first clarify this special case.

Decomposing the boundary terms in (2.1) with respect to the boundary $\mathcal{S}$ according to subsection 2.2.2, we can read off the condition of the functional differentiability of $C[N, N^e]$ [11]: the lapse and the shift are vanishing on $\mathcal{S}$ and the induced volume $(n-1)$-form $\varepsilon_{e_1\dots e_{n-1}}$ is fixed on $\mathcal{S}$. It is straightforward to check that the boundary condition $\delta\varepsilon_{e_1\dots e_{n-1}} = 0$ is preserved by the evolution equations with shifts and lapses vanishing on $\mathcal{S}$. Thus the quasi-local Hamiltonian phase space $T^*\mathcal{Q}(\Sigma)$ is split into disjoint sectors $T^*\mathcal{Q}(\Sigma, \varepsilon_{e_1,\dots,e_{n-1}})$, labeled by the value of the volume form on $\mathcal{S}$. The constraint functions are differentiable in the directions tangential to these sectors, but not in the directions transversal to them. The Poisson bracket of any two constraint functions $C[N, N^e]$ and $C[\bar N, \bar N^e]$, 'parameterized' by lapses and shifts that are vanishing on $\mathcal{S}$, is

$$
\Big\{C\big[N, N^a\big], C\big[\bar N, \bar N^a\big]\Big\} = C\big[\bar N^e D_e N - N^e D_e \bar N, N D^a \bar N - \bar N D^a N - [N, \bar N]^a\big]. \quad (2.11)
$$

Furthermore, the new smearing fields $\bar N^e D_e N - N^e D_e \bar N$ and $N D^a \bar N - \bar N D^a N - [N, \bar N]^a$ are also vanishing on the boundary $\mathcal{S}$. Therefore, the constraints close to a Poisson algebra $\mathcal{C}$.

Geometrically $N|_{\mathcal{S}} = 0$, $N^a|_{\mathcal{S}} = 0$ correspond to an evolution vector field $\xi^a = t^a N + N^a$ in the spacetime that is vanishing on $\mathcal{S}$, and hence the 1-parameter family of diffeomorphisms ϕ_t generated by ξ^a leaves $\mathcal{S}$ fixed *pointwise*. This ϕ_t maps Σ into a family Σ_t of Cauchy surfaces for the *same* globally hyperbolic domain $D(\Sigma)$ with the same boundary $\partial\Sigma_t = \mathcal{S}$. According to Bergmann [18], the gauge-invariant content of general relativity is the *spacetime geometry*, and hence any two sets of information that specify the same spacetime geometry must be considered to be gauge equivalent. In particular, two Cauchy data sets determining the same globally hyperbolic domain are gauge equivalent in this sense. (For different interpretations see e.g. [19, 20].) Therefore, the evolution vector fields ξ^a that are vanishing at $\mathcal{S}$ are precisely the generators of *gauge motions* of the actual quasi-local state in the *spacetime*.

2.3.2 The algebra of the basic Hamiltonians

If in the quasi-local Lagrangian phase space we choose the Lagrangian $L := \frac{1}{2\kappa}\int_\Sigma (R - 2\lambda + \chi_{ab}\chi^{ab} - \chi^2)N\sqrt{|h|}\mathrm{d}^n x$, then for the basic Hamiltonian we obtain

$$\begin{aligned} H_0\bigl[K^e\bigr] :=& C\bigl[K^e\bigr] + \int_\Sigma 2D_a\Bigl(\tilde{p}^{ab}h_{bc}N^c\Bigr)\mathrm{d}^n x = \\ =& C\bigl[K^e\bigr] - \frac{1}{\kappa}\oint_{\mathcal{S}} K^a\Bigl(-v_a t_b Q_c{}^{cb} + A_a\Bigr)\mathrm{d}\mathcal{S}. \end{aligned} \tag{2.12}$$

Thus we already have a nontrivial a priori Hamiltonian boundary term, in which both $v_a t_b Q_c{}^{cb}$ and A_a depend on the actual choice for the normals (t^a, v^a) of $\mathcal{S}$. This Hamiltonian can be made $2 + (n-1)$-covariant if K^e is restricted to be tangent to $\mathcal{S}$ and, to cure the $SO(1,1)$-gauge dependence of the connection 1-form, if $\delta_e K^e = 0$ is required.

In fact [11], evaluating the boundary terms in the total variation of H_0 we obtain that H_0 is functionally differentiable if the lapse is vanishing on $\mathcal{S}$, the shift is tangential to $\mathcal{S}$, and the volume $(n-1)$-form is fixed on $\mathcal{S}$. However, this boundary condition is preserved by the evolution equations precisely when $\delta_e N^e = 0$ is satisfied. With these boundary conditions the basic Hamiltonians form a Poisson algebra $\mathcal{H}_0$, in which the quasi-local constraint algebra $\mathcal{C}$ is an ideal. By evaluating the basic Hamiltonian on the constraint surface we get a function on the algebra $\mathcal{H}_0/\mathcal{C}$ of observables, which provides a representation of the Lie algebra of the δ_e-divergence-free vector fields on $\mathcal{S}$. Though the observable $O[N^e] := -\frac{1}{\kappa}\oint_{\mathcal{S}} N^e A_e \mathrm{d}\mathcal{S}$ behaves as angular momentum in certain special situations (see [11, 21]), but this can be non-zero even in Minkowski spacetime. This shows that the boundary term of H_0 should probably be present in the 'ultimate' Hamiltonian, but still further terms are needed.

Geometrically, $N|_{\mathcal{S}} = 0$, $v_a N^a|_{\mathcal{S}} = 0$ correspond to evolution vector fields *tangential* to $\mathcal{S}$ on $\mathcal{S}$. The corresponding 1-parameter family of diffeomorphisms still maps $D(\Sigma)$ onto itself and preserves the boundary $\mathcal{S}$, but not pointwise. Its action on $\mathcal{S}$ preserves the volume $(n-1)$ form. Thus H_0 is certainly not the 'ultimate' Hamiltonian, it is only an improved version of the constraint functions.

2.3.3 On the differentiability of the 'improved' basic Hamiltonian

The 'bad' gauge dependence of the basic Hamiltonian (2.12) can be improved slightly by hand by adding $N\nu = K^a t_a v_b Q_c{}^{cb}$ to the integrand of the boundary integral. (Here $\nu := \nu_{ab}q^{ab}$, the trace of the extrinsic curvature of $\mathcal{S}$ in Σ.) The resulting expression,

$$H_1\big[K^e\big] := C\big[K^e\big] - \frac{1}{\kappa}\oint_{\mathcal{S}} K^a\Big({}^\perp\varepsilon_{ab}Q_c{}^{cb} + A_a\Big)\mathrm{d}\mathcal{S}, \tag{2.13}$$

has been derived in different forms by several authors [22, 23, 24] and used [25] to define quasi-local energy.[1] Here the first term in the boundary integral became $2+(n-1)$ covariant, but the second term still depends on the $SO(1,1)$ boost gauge. To cure this dependence, we still must require $\delta_e K^e = 0$. In subsection 4.2 we will see that the boundary term of (2.13) emerges naturally among the boundary terms in the calculation of the Poisson bracket of two constraint functions (or Hamiltonians). Moreover, in that context there is a natural way of curing its $SO(1,1)$ boost-gauge dependence. On the other hand, as we will see, it does not seem to represent correctly the 'composition law' of the lapses and shifts.

Calculating the total variation of H_1, we can determine the condition of its functional differentiability. However, it is enough to calculate the total variation of the 'correction term' $N\nu$ and to use the expression (4.2) of [11] for the total variation $\delta H_0[K^e]$ of the basic Hamiltonian. The total variation of $N\nu\sqrt{|q|}$ is

$$\begin{aligned}\delta\big(N\nu\sqrt{|q|}\big) = \Big(&\nu\delta N + \frac{1}{2}Nv^e\big(D_e\delta h_{ab}\big)q^{ab} + \frac{1}{2}\nu N q^{ab}\delta q_{ab} + \\ &+\delta_a\big(N\delta v^a\big) - \big(\Delta_a N\big)\delta v^a - \nu N v_a\delta v^a\Big)\sqrt{|q|},\end{aligned}$$

where we used decomposition (2.4). This, together with $\delta H_0[K^e]$, yields

$$\begin{aligned}\delta H_1\big[N,N^e\big] =& C\big[\delta N,\delta N^e\big] + \int_\Sigma\Big(\frac{\delta C[N,N^e]}{\delta h_{ab}}\delta h_{ab} + \frac{\delta C[N,N^e]}{\delta\tilde p^{ab}}\delta\tilde p^{ab}\Big)\mathrm{d}^n x - \\ &-\frac{1}{\kappa}\oint_{\mathcal{S}}\Big\{\ \nu\,\delta N + \big(A_e - \tau v_e\big)\delta N^e + v_e N^e A_a\delta v^a - \tau v_e N^e v_a\delta v^a + \\ &\qquad+\frac{1}{2}\Big(-\nu^{ab}N + \tau^{ab}v_e N^e + \\ &\qquad\quad+\big(\nu N - \tau v_e N^e + v^e D_e N + \chi_{cd}v^c v^c v_e N^e\big)q^{ab}\Big)\delta q_{ab}\Big\}\mathrm{d}\mathcal{S}.\end{aligned}$$

Thus if the variations of the lapse and the shift were independent of the variations of the canonical variables, then the differentiability of $H_1[K^e]$ with respect to the metric h_{ab} could be ensured by keeping the whole n-metric fixed on $\mathcal{S}$: $\delta h_{ab}|_{\mathcal{S}} = 0$. However, this condition is not $2+(n-1)$-covariant, and from the compatibility of this boundary condition with the evolution equation for h_{ab} it follows that K^e on $\mathcal{S}$ must satisfy $v^c v^d\nabla_{(c}K_{d)} = 0$, $\Pi^c_a v^d\nabla_{(c}K_{d)} = 0$ and $\Pi^c_a\Pi^d_b\nabla_{(c}K_{d)} = 0$, which are conditions on the derivative of the lapse and shift in the direction v^a normal to $\mathcal{S}$, too. Another possibility is that the induced metric q_{ab} on $\mathcal{S}$ is fixed and the shift is tangent to $\mathcal{S}$. Apparently, this is a weaker condition for (N,N^a) than what we had in subsection 2.3.2. However, $v_e N^e|_{\mathcal{S}} = 0$ is invariant with respect to the $SO(1,1)$ transformation of the normals (t^a, v^a) only if we require $N|_{\mathcal{S}} = 0$, too, i.e. we arrived back to the basic Hamiltonian. Hence, we

[1] The same terms also appear in the general expression of the quasi-local quantities based on Møller's boost-gauge invariant, but still $O(1,n)$ gauge-dependent superpotential, and hence in the spinorial expressions based on the Nester–Witten 2-form in 3+1 dimensions, too. For details see the forthcoming updated version of [8].

conclude that *the Hamiltonian (2.13) could be the 'ultimate' quasi-local Hamiltonian only if the lapse and shift are not independent of the canonical variables.* Therefore, according to our expectation in subsection 2.1, the lapse and the shift should satisfy a certain linear differential equation on $\mathcal{S}$. In subsection 4.1 we derive such an equation, but to motivate those investigations first we study the quasi-local canonical formulation of a single real scalar field.

3 Illustration: Matter fields

3.1 Conserved quantities and flux integrals for general matter fields

Let the matter fields be described by the symmetric energy-momentum tensor T_{ab}, which is divergence free if the field equations are satisfied. Let K^e be any vector field, Σ a smooth compact spacelike hypersurface with smooth boundary $\mathcal{S} := \partial\Sigma$, and let us form the integral

$$\mathtt{Q}_\Sigma\big[K^e\big] := \int_\Sigma K_a T^{ab} \frac{1}{n!}\varepsilon_{be_1\dots e_n}. \tag{3.1}$$

Let ξ^e be another, arbitrary smooth vector field on M, define Σ_t to be the 1-parameter family of hypersurfaces by Lie dragging Σ along the integral curves of ξ^e such that $\Sigma_0 = \Sigma$ and form the 1-parameter family of integrals (3.1) on these hypersurfaces. Then the derivative of these integrals with respect to the natural parameter t along the integral curves of ξ^e at $t = 0$ is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{Q}_\Sigma\big[K^e\big] = \int_\Sigma L_\xi\big(K_a T^{ab}\frac{1}{n!}\varepsilon_{be_1\dots e_n}\big) = \int_\Sigma \Big(T^{ab}\nabla_{(a}K_{b)} + \big(\nabla_a T^{ab}\big)K_b\Big)\xi^c t_c \mathrm{d}\Sigma \, + \\ + \int_\Sigma \nabla_a\Big(\xi^a T^{bc}K_c - \xi^b T^{ac}K_c\Big)\frac{1}{n!}\varepsilon_{be_1\dots e_n}.\end{aligned}$$

However, the integrand of the second integral on the right can be rewritten into the exact n-form $-\frac{1}{(n-1)!}\nabla_{[e_1}(\varepsilon_{e_2\dots e_{n-1}]ab}\xi^a T^{bc}K_c)$, and hence by the Stokes theorem it can be converted into a boundary integral. Thus finally we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{Q}_\Sigma\big[K^e\big] = \int_\Sigma \Big(T^{ab}\nabla_{(a}K_{b)} + \big(\nabla_a T^{ab}\big)K_b\Big)\xi^c t_c \mathrm{d}\Sigma + \oint_{\mathcal{S}} \xi^{a\perp}\varepsilon_{ab}T^{bc}K_c \mathrm{d}\mathcal{S}. \tag{3.2}$$

Therefore, if the energy-momentum tensor is divergence free, there are two roots of the non-conservation of the quantity $\mathtt{Q}_\Sigma[K^e]$: The non-Killing nature of the vector field K^a and the boundary integral.

If K^a is a Killing field, then the vanishing of the right hand side of (3.2) can be expected only for ξ^a tangent to $\mathcal{S}$. The hypersurfaces Σ_t that such a ξ^a generates are such that the boundaries of all these coincide, $\partial\Sigma_t = \mathcal{S}$, and they are simply other Cauchy surfaces for the same globally hyperbolic domain $D(\Sigma)$. Therefore, the $\mathtt{Q}_\Sigma[K^e]$ for Killing K^e must in fact be conserved for ξ^e tangential to $\mathcal{S}$ on $\mathcal{S}$. For example, if (M, g_{ab}) is the Minkowski spacetime with Cartesian coordinates $\{x^{\underline{a}}\}$, $\underline{a} = 0,\dots,n$, then the general Killing field has the form $K_e = T_{\underline{a}}\nabla_e x^{\underline{a}} + M_{\underline{a}\underline{b}}(x^{\underline{a}}\nabla_e x^{\underline{b}} - x^{\underline{b}}\nabla_e x^{\underline{a}})$ for some constants $T_{\underline{a}}$

and $M_{\underline{a}\,\underline{b}} = M_{[\underline{a}\,\underline{b}]}$. Then the coefficients of these constants in $\mathtt{Q}_\Sigma[K^e] =: T_{\underline{a}}\,\mathtt{P}^{\underline{a}} + M_{\underline{a}\,\underline{b}}\,\mathtt{J}^{\underline{a}\,\underline{b}}$ define the quasi-local energy-momentum and angular momentum of the matter fields. These are conserved during the evolution with *any* ξ^e being tangent to $\mathcal{S}$ at $\mathcal{S}$, and transform in the correct, expected way under Poincaré transformations of the Cartesian coordinates. Hence the quasi-local quantities can be thought of as being associated with $\mathcal{S}$ or with the whole Cauchy development $D(\Sigma)$ of Σ.

To understand the meaning of the boundary integral in (3.2), suppose that ξ^e is not tangent to $\mathcal{S}$. Since the area 2-form ${}^\perp\varepsilon_{ab}$ annihilates the part of ξ^e tangential to $\mathcal{S}$, without loss of generality we may assume that ξ^e is orthogonal to $\mathcal{S}$. Let B denote the union of the boundaries $\partial\Sigma_t$ for all $|t| < \epsilon$ for some positive ϵ, i.e. the hypersurface that $\mathcal{S}$ sweeps out by Lie dragging along the integral curves of ξ^e. (This B is a smooth, regular hypersurface only if ξ^e is nowhere vanishing on $\mathcal{S}$. At the zeros of ξ^e the boundaries $\partial\Sigma_t$ intersect each other, and at these points B collapses to $(n-1)$ dimensional.) Then, by construction, $\xi^{a\perp}\varepsilon_{ab}$ is a (not normalized) normal 1-form to the (regular parts of) B on $\mathcal{S}$. Thus, the integrand of the boundary integral on the right hand side of (3.2) is the flux density of the current $T^{ab}K_b$ through B at $\mathcal{S}$ weighted by the 'length' of ξ^e. Therefore, for small enough Δt, $\oint_{\mathcal{S}} \xi^{a\perp}\varepsilon_{ab}T^{bc}K_c \mathrm{d}\mathcal{S}\Delta t$ is the *flux of the current* $T^{ab}K_b$ *through* B *between* $\partial\Sigma_0$ *and* $\partial\Sigma_{\Delta t}$. The root of the non-conservation of the quasi-local quantities $\mathtt{Q}_\Sigma[K^e]$ even for Killing K^e is that the actual system, surrounded at a given instant by $\mathcal{S}$, is *not* closed, and there can be non-trivial incoming and outgoing flows of energy-momentum and angular momentum.

In particular, if K^e is the time translational Killing field, $K_e = \nabla_e x^0$, then $\mathtt{Q}_\Sigma[K^e] = \mathtt{P}^0$, the quasi-local energy. If T^{ab} satisfies the dominant energy condition, then this is non-negative (and zero if and only if T^{ab} is vanishing on $D(\Sigma)$). Then by (3.2) $\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{P}^0$ is non-negative for outward pointing (i.e. for which $v_e\xi^e < 0$) spacelike or null ξ^e, non-positive for inward pointing (i.e. $v_e\xi^e > 0$) spacelike or null ξ^e, and does not have a definite sign for timelike ξ^e. In the first case only the incoming energy flow can cross B, yielding energy gain; in the second only the outgoing energy flow can cross B, yielding energy loss; while in the case of timelike B, both incoming and outgoing energy flows may be present.

As a conclusion, first, a distinction between evolution vector fields ξ^e generating the (e.g. time) evolution of the state and the generators of the quasi-local (conserved) quantities K^e must be made. (This view was already adopted already both for matter fields in [8, 26] and for gravitational fields that are asymptotically flat at spatial infinity in [6, 7].) Moreover, the boundary integral appearing in the 'time' derivative of the 'conserved' quantities describes the flux of the incoming and outgoing energy-momentum and angular momentum flows. We will see in subsection 3.2.2 that a detailed and systematic quasi-local Hamiltonian analysis of a single real scalar field exactly reproduces the result (3.2), where the boundary integral emerges as the boundary term in the Poisson bracket of two Hamiltonians. Though the gravitational 'field' does not have any well-defined energy-momentum density but admits a Hamiltonian formulation, an analogous result may be expected for the gravitational 'field' as well: the Poisson boundary term must have a physical meaning (and hence must be gauge invariant) for appropriately defined 'quasi-symmetry generators' K^e on $\mathcal{S}$.

3.2 Quasi-local Hamiltonian description of the scalar field

3.2.1 The quasi-local phase space and the Hamiltonian

Let Φ be a real scalar field on M, whose dynamics in the spacetime is governed by the Lagrangian $\mathcal{L} := \frac{1}{2}g^{ab}(\nabla_a\Phi)(\nabla_b\Phi) - V$, where the potential $V = V(\Phi)$ is a given *algebraic* function of the scalar field. For the sake of concreteness, we may assume that this has the form $V = \frac{1}{2}m^2\Phi^2 + \frac{1}{4}\mu\Phi^4$, i.e. the scalar field is of rest-mass m and μ is its self-interaction parameter. The covariant field equation and the energy-momentum tensor, respectively, are

$$\nabla_a\nabla^a\Phi + \frac{\partial V}{\partial\Phi} = 0, \tag{3.3}$$

$$T_{ab} = \bigl(\nabla_a\Phi\bigr)\bigl(\nabla_b\Phi\bigr) - \frac{1}{2}g_{ab}\bigl(\nabla_e\Phi\bigr)\bigl(\nabla^e\Phi\bigr) + g_{ab}V. \tag{3.4}$$

T_{ab} with the explicit form of the potential V above satisfies the dominant energy condition precisely when $\mu \geq 0$.

The basis of the quasi-local canonical formulation of the theory of scalar field is the quasi-local configuration space $\mathcal{Q}(\Sigma)$, the space of the smooth real scalar fields on Σ satisfying certain, not-yet-specified boundary conditions. The quasi-local Hamiltonian phase space is its 'cotangent bundle' $T^*\mathcal{Q}(\Sigma)$, endowed with its natural symplectic structure. The canonical momenta are scalar densities $\tilde\Pi$ on Σ. Using the Lagrangian $L : T\mathcal{Q}(\Sigma) \to \mathbb{R}$, defined by $L := \int_\Sigma \mathcal{L}N\sqrt{|h|}\mathrm{d}^n x$ and considered to be the function of the Lagrange variables $(\Phi, \dot\Phi)$, the standard canonical formalism yields for the momenta that $\tilde\Pi = t^a(\nabla_a\Phi)\sqrt{|h|} = \frac{1}{N}(\dot\Phi - N^e D_e\Phi)\sqrt{|h|}$ and for the Hamiltonian $H : T^*\mathcal{Q}(\Sigma) \to \mathbb{R}$, introduced by $H := \int_\Sigma(\tilde\Pi\dot\Phi - \mathcal{L}N\sqrt{|h|})\mathrm{d}^n x$, that

$$H = \int_\Sigma \Bigl\{N\Bigl(\frac{1}{2}\frac{\tilde\Pi^2}{|h|} - \frac{1}{2}h^{ab}\bigl(D_a\Phi\bigr)\bigl(D_b\Phi\bigr) + V\Bigr)\sqrt{|h|} + N^e\bigl(D_e\Phi\bigr)\tilde\Pi\Bigr\}\mathrm{d}^n x. \tag{3.5}$$

A straightforward calculation shows that the coefficient of N is just the energy density part $\mu := T_{ab}t^a t^b$ and the coefficient of N^e is just the momentum density part $J_e := P^a_e T_{ab}t^b$ of the symmetric energy-momentum tensor. Thus we can also write $H = \int_\Sigma K^a T_{ab}t^b \mathrm{d}\Sigma$, where $K^a = Nt^a + N^a$. If more than one Hamiltonians 'parameterized' by different lapse-shift pairs are considered, then to indicate which lapse-shift is used we write the Hamiltonian as $H[N, N^e]$ or $H[K^e]$.

Since H depends on the 'parameters' N and N^e, the spatial metric h_{ab} and the momentum variable $\tilde\Pi$ *algebraically*, H is functionally differentiable with respect to them, independently of the boundary conditions on $\mathcal{S}$. (Though in the present context the functional differentiability with respect to N, N^e and h_{ab} does not have any significance, in subsection 4.1.5, where we consider the Einstein–scalar system, h_{ab} will be the gravitational configuration variable, and hence the functional differentiability with respect to h_{ab} will be important.) The corresponding functional derivatives themselves are

$$\frac{\delta H}{\delta N} = \mu\sqrt{|h|}, \quad \frac{\delta H}{\delta N^a} = J_a\sqrt{|h|}, \quad \frac{\delta H}{\delta h_{ab}} = \frac{1}{2}N\sigma^{ab}\sqrt{|h|}, \tag{3.6}$$

where $\sigma_{ab} := T_{cd}P^c_a P^d_b$, the spatial stress part of the symmetric energy-momentum tensor (3.4), and

$$\frac{\delta H}{\delta\tilde\Pi}=N\frac{\tilde\Pi}{\sqrt{|h|}}+N^eD_e\Phi. \tag{3.7}$$

Nevertheless, the condition of the functional differentiability with respect to Φ is

$$\oint_{\mathcal{S}}v^a\Big(N_a\Pi-N\big(D_a\Phi\big)\Big)\delta\Phi\mathrm{d}\mathcal{S}=0. \tag{3.8}$$

(Here Π is the 'de-densitized' canonical momentum: $\tilde\Pi=:\Pi\sqrt{|h|}$.) (3.8) can be ensured either by fixing the configuration variable Φ on $\mathcal{S}$, $\delta\Phi|_{\mathcal{S}}=0$, or by requiring the vanishing of the coefficient of $\delta\Phi$ in (3.8). Under any of these conditions H is functionally differentiable, and its functional derivative with respect to the configuration variable is

$$\frac{\delta H}{\delta\Phi}=-D_a\Big(N^a\tilde\Pi-N\big(D^a\Phi\big)\sqrt{|h|}\Big)+N\frac{\partial V}{\partial\Phi}\sqrt{|h|}. \tag{3.9}$$

Then the canonical equations of motion are

$$\dot\Phi=\frac{\delta H}{\delta\tilde\Pi}=N\Pi+N^aD_a\Phi, \tag{3.10}$$

$$\dot{\tilde\Pi}=-\frac{\delta H}{\delta\Phi}=-D_a\Big(N\sqrt{|h|}D^a\Phi-N^a\tilde\Pi\Big)-N\frac{\partial V}{\partial\Phi}\sqrt{|h|}. \tag{3.11}$$

The first is equivalent to the definition of the time derivative of Φ, while the second to the field equation (3.3).

Returning to the boundary conditions, the first, $\delta\Phi|_{\mathcal{S}}=0$, is analogous to the Dirichlet boundary condition in electrostatics. However, according to our requirement (ii) in subsection 2.1.1, the evolution equation (3.10) must preserve this, and hence we obtain that at $\mathcal{S}$ the canonical variables must satisfy

$$N\Pi+N^aD_a\Phi=0. \tag{3.12}$$

Thus, the canonical momentum (weighted by the lapse) must be linked to the derivative of Φ in the direction of the shift. In particular, for vanishing shift $\tilde\Pi$ must be vanishing on $\mathcal{S}$. The other possible boundary condition coming from (3.8) is the requirement of the vanishing of the coefficient of $\delta\Phi$ on $\mathcal{S}$:

$$v^aN_a\Pi-Nv^aD_a\Phi=0. \tag{3.13}$$

Thus, the normal directional derivative of Φ (weighted by the lapse) is linked to the canonical momentum on $\mathcal{S}$. This is analogous to the (generalized) Neumann-type boundary condition in electrostatics. (The Dirichlet- and Neumann-type boundary conditions appear naturally in a covariant phase-space context too. For details, see [27, 28].)

3.2.2 The Poisson boundary term and the flux integral

Let (N,N^e) and $(\bar N,\bar N^e)$ be two lapse-shift pairs, assume that both $H[N,N^a]$ and $H[\bar N,\bar N^a]$ are differentiable and let us calculate the Poisson bracket of two Hamiltonians parameterized by them. By integration by parts, a direct calculation yields that it is

$$
\begin{aligned}
&\Big\{H\big[N,N^e\big],H\big[\bar N,\bar N^e\big]\Big\}= \qquad (3.14)\\
&=H\Big[\bar N^aD_aN-N^aD_a\bar N,ND^a\bar N-\bar ND^aN-\big[N,\bar N\big]^a\Big]+\\
&+\int_\Sigma\Big(ND_{(a}\bar N_{b)}-\bar ND_{(a}N_{b)}\Big)\sigma^{ab}\mathrm{d}\Sigma-\\
&-\oint_{\mathcal S}v_a\Big\{\big(N^a\bar N^b-\bar N^aN^b\big)J_b+\big(\bar NN_b-N\bar N_b\big)\sigma^{ab}+\big(\bar NN^a-N\bar N^a\big)\Pi^2\Big\}\mathrm{d}\mathcal{S}.
\end{aligned}
$$

Note that the new lapse and shift that parameterize the Hamiltonian on the right are exactly those that appeared in the constraint algebra of Einstein's theory (see subsection 2.3.1). But in addition to the Hamiltonian H the spatial integral of the spatial stress, contracted with the Killing operators acting on the shift vectors (and weighted by the lapses), also appears. These operators can be replaced by the *spacetime* Killing operators acting on appropriately defined *spacetime* vector fields. Indeed, let us fix a foliation of the spacetime with lapse M and a compatible evolution vector field $\xi^e:=Mt^e+M^e$, where t^e is the future pointing unit timelike normal of the leaves of this foliation, and define $K^a:=Nt^a+N^a$ and $\bar K^a:=\bar Nt^a+\bar N^a$. Then the complete $n+1$ decomposition of the Killing operator $\nabla_{(a}\bar K_{b)}$ with respect to this foliation and evolution vector field ξ^e is

$$
\begin{aligned}
Mt^ct^d\nabla_{(c}\bar K_{d)}&=\dot{\bar N}+\bar N^aD_aM-M^aD_a\bar N, &(3.15)\\
2Mh^{ac}t^d\nabla_{(c}\bar K_{d)}&=\dot{\bar N}^a+MD^a\bar N-\bar ND^aM-\big[M,\bar N\big]^a, &(3.16)\\
P^c_aP^d_b\nabla_{(c}\bar K_{d)}&=\bar N\chi_{ab}+D_{(a}\bar N_{b)}, &(3.17)
\end{aligned}
$$

where $\dot{\bar N}$ and $\dot{\bar N}^a$ denote the time derivative of $\bar N$ and $\bar N^a$ with respect to ξ^e, respectively, introduced in subsection 2.2.1. Note that while the normal-normal and normal-tangential parts of the spacetime Killing operator depend on M and M^a, its spatial projection does not. It is well defined even on a single spacelike hypersurface. Thus, by (3.17), the integrand of the n-dimensional integral on the right-hand side of (3.14) is $\sigma^{ab}(N\nabla_{(a}\bar K_{b)}-\bar N\nabla_{(a}K_{b)})$.

On the other hand, contrary to the bulk terms, the boundary integral (which we call the Poisson boundary term) apparently contains the canonical momentum explicitly, and not only through the various parts of the symmetric energy momentum tensor. However, if we take into account any of the boundary conditions (3.12) and (3.13), then the Poisson boundary term can be rewritten purely in terms of the energy-momentum tensor. In fact, if (3.12) holds (both for (N,N^a) and $(\bar N,\bar N^a)$), then by $\bar N\Pi^2=-\bar N^a(D_a\Phi)\Pi=-\bar N^aJ_a$ the first and the third terms in the boundary integral of (3.14) cancel each other, and there remains only $v_a\sigma^{ab}(\bar NN_b-N\bar N_b)$. Similarly, using the explicit form of the spatial stress σ_{ab}, we can write $\sigma^{ab}\bar NN_b=\bar NN^a\mu+N^a\bar N^bJ_b-N\bar NJ^a$. Then, however, it is straightforward to check that the integrand of the boundary integral is an expression of the energy-momentum tensor, and the final form of (3.14) is

$$
\begin{aligned}
&\Big\{H\big[N,N^e\big],H\big[\bar N,\bar N^e\big]\Big\}=\\
&=H\Big[\bar N^aD_aN-N^aD_a\bar N,ND^a\bar N-\bar ND^aN-\big[N,\bar N\big]^a\Big]+\\
&+\int_\Sigma\Big(N\nabla_{(a}\bar K_{b)}-\bar N\nabla_{(a}K_{b)}\Big)\sigma^{ab}\mathrm{d}\Sigma+\oint_{\mathcal S}K^{a\perp}\varepsilon_{ac}T^c{}_b\bar K^b\mathrm{d}\mathcal{S}. \qquad (3.18)
\end{aligned}
$$

Using the boundary condition it is easy to check that the boundary integral is anti-symmetric in $K^a\bar K^b$, as it should be because every other term in (3.18) changes sign if we interchange (N, N^a) and $(\bar N, \bar N^a)$. Similarly, if (3.13) holds, then the last term in the boundary integral in (3.14) is vanishing, and $v_a\sigma^{ab}\bar N N_b = v_a N^a\bar N\mu + v_a\bar N^a N^b J_b - \bar N N v^b J_b$ holds. Using this expression, (3.14) again takes the form (3.18).

Recalling that in the spacetime picture the Hamiltonian $H[N, N^a]$ is the flux integral of the Lorentz-covariant current $T^{ab}K_b$, it is natural to ask for the spacetime-covariant form of (3.18), too. To derive this, let us decompose the Lie bracket $[K, \bar K]^a$ of the spacetime vector fields K^a and $\bar K^a$ with respect to the foliation and evolution vector field above. It is

$$\begin{aligned} \big[K, \bar K\big]^a t_a &= t^b t^c\Big(N\nabla_{(b}\bar K_{c)} - \bar N\nabla_{(b}K_{c)}\Big) + N^a D_a\bar N - \bar N^a D_a N, && (3.19)\\ \big[K, \bar K\big]^b P^a_b &= 2h^{ab}t^c\Big(N\nabla_{(b}\bar K_{c)} - \bar N\nabla_{(b}K_{c)}\Big) - \\ &\quad -\big(N D^a\bar N - \bar N D^a N\big) + \big[N, \bar N\big]^a. && (3.20) \end{aligned}$$

Thus *the new lapse and shift both in (2.11) and (3.14) appear as the lapse and shift parts of the Lie bracket of the spacetime vector fields up to the spacetime Killing operators.* Substituting these into (3.18) and using the notation $H[K^e] = H[N, N^e]$, we obtain

$$\begin{aligned} \Big\{H\big[K^e\big], H\big[\bar K^e\big]\Big\} &= -H\Big[\big[K, \bar K\big]^e\Big] + \int_\Sigma t^c\Big(K_c\nabla_{(a}\bar K_{b)} - \bar K_c\nabla_{(a}K_{b)}\Big)T^{ab}\mathrm{d}\Sigma + \\ &\quad + \frac{1}{2}\oint_{\mathcal S}\big(K^a\bar K^b - \bar K^a K^b\big)\,{}^\perp\varepsilon_{ac}T^c{}_b\mathrm{d}\mathcal S. \qquad (3.21) \end{aligned}$$

Therefore, the quasi-local Hamiltonians of the real scalar field do *not* form a Poisson algebra. The two roots of this failure are the non-Killing nature of the vector fields K^a and $\bar K^a$ and the boundary integral. The latter is precisely the boundary integral of (3.2). Our aim is to recover the whole of (3.2).

To do this, let us calculate the time derivative of $H[\bar N, \bar N^a]$ with respect to ξ^a in the spacetime. It is

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}H\big[\bar N, \bar N^a\big] &= \int_\Sigma\Big(\mu\dot{\bar N} + J_a\dot{\bar N}^a + \frac{1}{2}\bar N\sigma^{ab}\dot h_{ab}\Big)\mathrm{d}\Sigma + \\ &\quad + \int_\Sigma\Big(\frac{\delta H[\bar N, \bar N^a]}{\delta\Phi}\dot\Phi + \frac{\delta H[\bar N, \bar N^a]}{\delta\tilde\Pi}\dot{\tilde\Pi}\Big)\mathrm{d}^n x = \\ &= \int_\Sigma\Big(\mu\dot{\bar N} + J_a\dot{\bar N}^a + \bar N\sigma^{ab}\big(M\chi_{ab} + D_{(a}M_{b)}\big)\Big)\mathrm{d}\Sigma + \\ &\quad + \Big\{H\big[M, M^a\big], H\big[\bar N, \bar N^a\big]\Big\}, \qquad (3.22) \end{aligned}$$

where in the first step we used the functional differentiability of $H[\bar N, \bar N^a]$, and in the second the canonical equations of motion with the Hamiltonian $H[M, M^a]$. Finally, by the expression (3.18) of the Poisson bracket and the projections (3.15)-(3.17) of the spacetime Killing operator, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}H\big[\bar N, \bar N^a\big] = \int_\Sigma\xi^c t_c T^{ab}\nabla_{(a}\bar K_{b)}\mathrm{d}\Sigma + \oint_{\mathcal S}\xi^a\,{}^\perp\varepsilon_{ac}T^{cb}\bar K_b\mathrm{d}\mathcal S. \qquad (3.23)$$

Thus we recovered (3.2), whose boundary integral appeared here as the Poisson boundary term.

4 The Poisson boundary terms in GR

4.1 The Poisson boundary terms

4.1.1 The formal Poisson brackets

Though in subsection 2.1.1 we defined the Poisson bracket for *functionally differentiable* functions on the phase space, we can define the *formal* Poisson bracket of any two constraint functions $C[N, N^e]$ and $C[\bar N, \bar N^e]$ by the integral of their *formal* functional derivatives, independently of their functional differentiability. A lengthy but straightforward calculation gives (or see [6, 11])

$$
\begin{aligned}
\Big\{C\big[N, N^a\big]\,, C\big[\bar N, \bar N^a\big]\Big\} = C\Big[&\bar N^e D_e N - N^e D_e \bar N\,,\, N D^a \bar N - \bar N D^a N - \big[N, \bar N\big]^a\Big] - \\
&- \oint_{\mathcal{S}} 2 v_a p^{ab}\Big(N D_b \bar N - \bar N D_b N - \big[N, \bar N\big]_b\Big)\mathrm{d}\mathcal{S} - \\
&- \oint_{\mathcal{S}} 2 p^{ab}\Big(v_e N^e D_a \bar N_b - v_e \bar N^e D_a N_b\Big)\mathrm{d}\mathcal{S} - \\
&- \oint_{\mathcal{S}} \frac{1}{\kappa}\Big\{\frac{1}{2}\Big(R - 2\lambda + \chi^2 - \chi_{ab}\chi^{ab}\Big)\big(N\bar N^e - \bar N N^e\big)v_e - v^a R_{ab}\big(N\bar N^b - \bar N N^b\big) \\
&\quad + v^a\big(D_a N\big)\big(D_b \bar N^b\big) - \big(D^b N\big)\big(D_b \bar N_a\big)v^a - \\
&\quad - v^a\big(D_a \bar N\big)\big(D_b N^b\big) + \big(D^b \bar N\big)\big(D_b N_a\big)v^a\Big\}\mathrm{d}\mathcal{S}.
\end{aligned}
\tag{4.1}
$$

A well-known highly non-trivial property of the constraint functions is that in their formal Poisson bracket, the genuine n-dimensional integral is also a constraint function (with the new lapse $\bar N^e D_e N - N^e D_e \bar N$ and the new shift $N D^a \bar N - \bar N D^a N - \big[N, \bar N\big]^a$), and the remaining terms are all boundary integrals. It might also be interesting to note that the first two terms on the right together is just the basic Hamiltonian of subsection 2.3.2 parameterized by the new lapse and shift.

4.1.2 The main idea

We learnt in subsection 3.2.2 that the Poisson boundary term in $\{H[\xi^a], H[\bar K^a]\}$ describes, at least for appropriately chosen Killing fields $\bar K^a$, the infinitesimal flux of energy-momentum and angular momentum flows through the hypersurface that is generated by Lie dragging $\mathcal{S}$ along the integral curves of ξ^a. However, if we could expect that the Poisson boundary term has a physical meaning in general relativity too, then (in addition to the requirement of the functional differentiability of the Hamiltonian and the compatibility of the boundary conditions and the evolution equations) we would have a further condition that we could use to find the 'ultimate' Hamiltonian boundary term and the boundary conditions.

Thus suppose for a moment that we already have the 'ultimate' Hamiltonian boundary term and the boundary conditions both for the canonical variables and the lapse and the shift; and hence $H[N, N^a]$, given by (1.3), is functionally differentiable. Then the

Poisson bracket of two such Hamiltonians is precisely the *formal* Poisson bracket of the two *constraints* with the same lapses and shifts, which is already given explicitly by (4.1). However, if our expectation is correct, then this Poisson bracket must be the sum of the 'correct' Hamiltonian (parameterized by the new lapse and shift) and another physical quantity (being analogous to the energy-momentum and angular momentum fluxes). Consequently, since both are gauge invariant, the Poisson boundary term *must* also be gauge invariant. In particular, this Poisson boundary term

1. should depend only on $N|_{\mathcal{S}}$, $\bar{N}|_{\mathcal{S}}$, $N^a|_{\mathcal{S}}$ and $\bar{N}^a|_{\mathcal{S}}$, but not on their normal derivatives, e.g. on $v^eD_eN|_{\mathcal{S}}$ or $v^eD_eN^a|_{\mathcal{S}}$;
2. should depend only on the geometry of $\mathcal{S}$, but not on the geometry of Σ at its boundary $\mathcal{S}$;
3. must be $2+(n-1)$-covariant and, in particular, it must be independent of the actual choice for the normals (t^a, v^a) to $\mathcal{S}$.

Therefore, we must check whether or not the boundary terms in (4.1) satisfy these criteria. This will be done by rewriting it in a form adapted to $\mathcal{S}$, using the ideas and notions summarized in subsection 2.2.2.

4.1.3 The covariant form of the Poisson boundary term

Using the definitions of subsection 2.2.2, by a systematic decomposition of every tensor field and derivative operator according to $P^a_b = \Pi^a_b - v^a v_b$ we rewrite the integrand of every boundary integral in (4.1). Our ultimate aim is to obtain a $2+(n-1)$-covariant form and, in particular, in terms of the spacetime vector fields $K^e := Nt^e + N^e$ and $\bar{K}^e := \bar{N}t^e + \bar{N}^e$ rather than the individual lapses and shifts.

First, by a tedious but straightforward computation for the integrand I_1 of the first boundary integral in (4.1), we obtain

$$\begin{aligned}2\kappa I_1 = &\Big(K^e\delta_e\bar{K}^a - \bar{K}^e\delta_eK^a\Big)\big(\tau v_a - A_a\big) + \\ &+ \Big(\tau t_c A_d - A^b\big(\tau_{bc}t_d - \nu_{bc}v_d\big)\Big)\big(K^c\bar{K}^d - \bar{K}^cK^d\big) - \\ &- A_bA^{b\perp}\varepsilon_{cd}K^c\bar{K}^d + \\ &+ \Big(\big(\delta_e\bar{K}^a\big)t_at_bK^b - \big(\delta_eK^a\big)t_at_b\bar{K}^b\Big)A^e + \\ &+ \Big(\bar{N}v^eD_eN - Nv^eD_e\bar{N}\Big)\tau + \\ &+ \Big(v_eN^ev^aD_a\bar{N}_b - v_e\bar{N}^ev^aD_aN_b\Big)\big(A^b - \tau v^b\big).\end{aligned} \tag{4.2}$$

(To reproduce this formula (and the similar ones below), it seems useful to calculate first the projections of various quantities, e.g. $2\kappa v_a v_b p^{ab} = \chi_{ab}v^av^b + \chi = \tau_{ab}q^{ab} = \tau$, $2\kappa v_a p^{ab}q_{bc} = A_c$ or $2\kappa p^{cd}q_{ca}q_{db} = \tau_{ab} - q_{ab}(\tau - \chi_{cd}v^cv^d)$. Note that $\chi_{ab}v^av^b$ cannot be expressed by quantities defined only on $\mathcal{S}$.)

Similarly, the integrand I_2 of the second boundary integral is

$$
\begin{aligned}
2\kappa I_2 = & \Big(v_eK^e\Delta_a\bar K_b - v_e\bar K^e\Delta_aK_b\Big)\big(\tau^{ab}-\tau q^{ab}\big) + \\
&+\Big(v_eK^e\big(\Delta_a\bar K^a\big) - v_e\bar K^e\big(\Delta_aK^a\big)\Big)\chi_{cd}v^cv^d + \\
&+\Big(\tau_{ab}\tau^{ab}-\tau^2+\tau\chi_{ab}v^av^b - A_bA^b\Big)\,{}^\perp\varepsilon_{cd}K^c\bar K^d + \\
&+\Big(v_e\bar K^e\big(\Delta_aK_b\big)v^b - v_eK^e\big(\Delta_a\bar K_b\big)v^b\Big)A^a + \\
&+\Big(v_eK^ev^aD_a\bar N_b - v_e\bar K^ev^aD_aN_b\Big)\big(\tau v^b - A^b\big).
\end{aligned}
\tag{4.3}
$$

Before rewriting the integrand I_3 of the third boundary integral let us observe that the Ricci tensor and the curvature scalar appear in I_3 just like in the 'constraint parts' $v^av^bG_{ab}$ and $v^aG_{ab}\Pi^b_c$ of the Einstein tensor of the n-dimensional intrinsic (spatial) geometry (Σ, h_{ab}). Expressing these in terms of the curvature scalar ${}^{\mathcal S}R$ and the extrinsic curvature ν_{ab} of $\mathcal S$ (and its derivative $\delta_e\nu_{ab}$), a direct but quite lengthy calculation gives that

$$
\begin{aligned}
2\kappa I_3 = & -\lambda\,{}^\perp\varepsilon_{cd}K^c\bar K^d + \delta_a\Big(\big(\nu^{ab}-\nu q^{ab}\big)\big(N\bar N_b - \bar NN_b\big)\Big) + \\
&+\frac12\Big({}^{\mathcal S}R + \big(\nu_{ab}\nu^{ab}-\nu^2-\tau_{ab}\tau^{ab}+\tau^2\big)\Big){}^\perp\varepsilon_{cd}K^c\bar K^d + \\
&+v^a\big(D_aN\big)\Big(\Delta_b\bar K^b - \tau\bar N\Big) - v^a\big(D_a\bar N\big)\Big(\Delta_bK^b - \tau\bar N\Big) + \\
&+\Big(2A_aA^a - \tau\chi_{ab}v^av^b\Big){}^\perp\varepsilon_{cd}K^c\bar K^d + \\
&+\Big(\bar K^a\big(\delta_aK_b\big) - K^a\big(\delta_a\bar K_b\big)\Big)t^b\nu + \\
&+A_a\Big(K^a\bar K^b - \bar K^aK^b\Big)v_b\nu + \\
&+\big(\nu^{ab}-\nu q^{ab}\big)t_c\Big(\bar K^c\delta_aK_b - K^c\delta_a\bar K_b\Big) + \\
&+\big(\delta_e\bar K_a\big)\big(\delta^eK_b\big)\,{}^\perp\varepsilon^{ab} + \\
&+A^b\Big(\big(\delta_b\bar K_a\big)v^av_cK^c - \big(\delta_bK_a\big)v^av_c\bar K^c\Big) + \\
&+A^b\Big(\big(\delta_bK_a\big)t^at_c\bar K^c - \big(\delta_b\bar K_a\big)t^at_cK^c\Big) + \\
&+A^c\tau_{ca}t_b\big(K^a\bar K^b - \bar K^a\bar K^b\big).
\end{aligned}
\tag{4.4}
$$

Adding the three integrands and forming total δ_a-divergences, the resulting expression can be written in the form

$$
\begin{aligned}
2\kappa\big(I_1+I_2+I_3\big) = {} & \Big(\bar{K}^e\delta_e K_a - K^e\delta_e\bar{K}_a\Big)\,{}^{\perp}\varepsilon^{ab}Q^c{}_{cb} + \\
& + \big(\delta_e\bar{K}^a\big)\big(\delta^e K^b\big)\,{}^{\perp}\varepsilon_{ab} - \lambda\,{}^{\perp}\varepsilon_{ab}K^a\bar{K}^b + \\
& + \big(\delta_a A_b - \delta_b A_a\big)K^a\bar{K}^b + \\
& + \frac{1}{2}\Big({}^{\mathcal{S}}R + \tau_{ab}\tau^{ab} - \tau^2 - \nu_{ab}\nu^{ab} + \nu^2\Big)\,{}^{\perp}\varepsilon_{cd}K^c\bar{K}^d + \\
& + \big(\Delta_a\bar{K}_b\big)Q^{abc}\,{}^{\perp}\varepsilon_{cd}K^d - \big(\Delta_a K_b\big)Q^{abc}\,{}^{\perp}\varepsilon_{cd}\bar{K}^d + \\
& + \big(\Delta_b\bar{K}^b\big)\Big(v^e D_e N + v_e N^e\chi_{cd}v^c v^d - A_e N^e - Q^e{}_{ec}\,{}^{\perp}\varepsilon^{cd}K_d\Big) - \\
& - \big(\Delta_b K^b\big)\Big(v^e D_e\bar{N} + v_e\bar{N}^e\chi_{cd}v^c v^d - A_e\bar{N}^e - Q^e{}_{ec}\,{}^{\perp}\varepsilon^{cd}\bar{K}_d\Big) + \\
& + \delta_a\Big(\big(\bar{K}^a K^b - K^a\bar{K}^b\big)A_b + \big(\nu^{ab} - \nu q^{ab}\big)t^c\big(K_c\bar{K}_b - \bar{K}_c K_b\big)\Big).
\end{aligned}
\tag{4.5}
$$

Since the third line is just the contraction of the curvature of the connection δ_e in the normal bundle and the vector fields K^a and $\bar{K}^a$, moreover the fourth line is proportional to the trace of (2.7); one might attempt to rewrite (4.5) in a form containing the curvature $F^a{}_{bcd}$ of Δ_e. We show that this can indeed be done.

To get terms such as the right hand side of (2.8) and (2.9), let us rewrite the first as well as the fifth lines of (4.5) as total δ_e-divergences and terms with the derivative of the extrinsic curvature tensor. Re-expressing the second line in terms of the Δ_e-derivative operator we have

$$
\begin{aligned}
2\kappa\big(I_1+I_2+I_3\big) = {} & -\lambda\,{}^{\perp}\varepsilon_{cd}K^c\bar{K}^d - \big(\Delta^e K^a\big)\big(\Delta_e\bar{K}^b\big)\,{}^{\perp}\varepsilon_{ab} + \\
& + \frac{1}{2}\Big({}^{\mathcal{S}}R + \nu_{ab}\nu^{ab} - \nu^2 - \tau_{ab}\tau^{ab} + \tau^2\Big)\,{}^{\perp}\varepsilon_{cd}K^c\bar{K}^d + \\
& + \frac{1}{2}\Big(\delta_a A_b - \delta_b A_a + \tau_a{}^e\nu_{eb} - \tau_b{}^e\nu_{ea}\Big)\big(K^a\bar{K}^b - \bar{K}^a K^b\big) + \\
& + \Big(\delta_a Q^a{}_{ce} - \delta_c Q^a{}_{ae}\Big)\,{}^{\perp}\varepsilon^e{}_d\big(K^c\bar{K}^d - \bar{K}^c K^d\big) + \\
& + \big(\Delta_b\bar{K}^b\big)\Big(v^e D_e N + v_e N^e\chi_{cd}v^c v^d - A_e N^e\Big) - \\
& - \big(\Delta_b K^b\big)\Big(v^e D_e\bar{N} + v_e\bar{N}^e\chi_{cd}v^c v^d - A_e\bar{N}^e\Big) + \\
& + \delta_a\Big(\big(\bar{K}^a K^b - K^a\bar{K}^b\big)\big(A_b + {}^{\perp}\varepsilon_{bc}Q_e{}^{ec}\big) + \big(\bar{K}^e K_b - K^e\bar{K}_b\big)\,{}^{\perp}\varepsilon_{ef}Q^{abf} + \\
& \quad + \big(\nu^{ab} - \nu q^{ab}\big)t^c\big(K_c\bar{K}_b - \bar{K}_c K_b\big)\Big).
\end{aligned}
\tag{4.6}
$$

Comparing its second, third and fourth lines with (2.7)-(2.10), we find that these can be rewritten as

$$
\begin{aligned}
& \frac{1}{2}F^{ab}{}_{ab}\,{}^{\perp}\varepsilon_{cd}K^c\bar{K}^d + \frac{1}{2}\,{}^{\perp}\varepsilon_{ab}F^{ab}{}_{cd}K^c\bar{K}^d + F^{ab}{}_{bc}\,{}^{\perp}\varepsilon_{ad}\big(K^c\bar{K}^d - \bar{K}^c K^d\big) = \\
& = \frac{1}{8}K^a\bar{K}^b F^{cd}{}_{ef}\,{}^{\perp}\varepsilon_{gh}\delta^{efgh}_{abcd},
\end{aligned}
\tag{4.7}
$$

by means of which we arrive at our final expression for the formal Poisson bracket of two constraint functions:

$$
\begin{aligned}
&\Big\{C\big[N,N^a\big]\,,C\big[\bar N,\bar N^a\big]\Big\}=\\
&\qquad=C\Big[\bar N^eD_eN-N^eD_e\bar N\,,\,ND^a\bar N-\bar ND^aN-\big[N,\bar N\big]^a\Big]+\\
&\qquad+\frac{1}{\kappa}\oint_{\mathcal S}\Big\{\lambda\,{}^\perp\varepsilon_{ab}K^a\bar K^a+\big(\Delta^eK^a\big)\big(\Delta_e\bar K^b\big)\,{}^\perp\varepsilon_{ab}-\\
&\qquad\quad-\frac{1}{8}K^a\bar K^bF^{cd}{}_{ef}\,{}^\perp\varepsilon_{gh}\delta^{efgh}_{abcd}+\\
&\qquad\quad+\big(\Delta_bK^b\big)\Big(v^eD_e\bar N+v_e\bar N^e\chi_{cd}v^cv^d-\bar N^eA_e\Big)-\\
&\qquad\quad-\big(\Delta_b\bar K^b\big)\Big(v^eD_eN+v_eN^e\chi_{cd}v^cv^d-N^eA_e\Big)\Big\}\mathrm{d}\mathcal S.
\end{aligned}
\tag{4.8}
$$

Since the curvature $F^a{}_{bcd}$ is the pull back to $\mathcal S$ of the spacetime curvature 2-form ${}^MR^a{}_{bcd}$, in the physically important special case $n=3$ the curvature term reduces to $\frac{1}{4}K^a\bar K^b\varepsilon_{abcd}$ ${}^MR^{cd}{}_{ef}\varepsilon^{ef}$, and hence gives a Penrose-type charge integral of the spacetime curvature [29]. In a GHP spin frame (o^A,ι^A) adapted to $\mathcal S$ this takes the form $K^a\bar K^b\varepsilon_{A'B'}(\Psi_{ABCD}o^C\iota^D-\Phi_{ABC'D'}\bar o^{C'}\bar\iota^{D'}+\Lambda(o_A\iota_B+\iota_Ao_B))+c.c.$. Thus, in particular, it is only the Ψ_1, Ψ_2 and the Ψ_3, but not the Ψ_0 and Ψ_4 Weyl spinor components that are involved in the Poisson boundary term.

4.1.4 Boundary conditions from the gauge invariance of the Poisson boundary term

Clearly, the first three terms in the boundary integral of (4.8) are manifestly $2+(n-1)$-covariant; they depend only on the geometry of $\mathcal S$ and the value of the vector fields on $\mathcal S$ (but independent of the way in which they are extended off the boundary), and they are invariant with respect to the change of the actual normals (t^a,v^a) of $\mathcal S$. On the other hand, the last two lines contain 'bad' terms. Thus, we can ensure the gauge invariance of the Poisson boundary term (in the sense discussed in subsection 4.1.2) if *we require the vanishing of the Δ_e-divergence of the vector fields K^a* and $\bar K^a$. Obviously, $\Delta_aK^a=0$ is a $2+(n-1)$ covariant condition, and from $\Delta_aK^a=\delta_aK^a+Q^a{}_{ab}K^b=N\tau-v_aN^a\nu+\delta_a(\Pi^a_bN^b)$ it is clear that it has infinitely many solutions on $\mathcal S$: the condition $\Delta_aK^a=0$ specifies e.g. only the lapse N in terms of the still completely freely specifiable shift N^a.

To see the meaning of this condition, let us rewrite this into the form $q^{ab}\Pi^c_a\Pi^d_b$ $\nabla_{(c}K_{d)}=0$. This is one of the $\frac{1}{2}n(n-1)$ projected parts of the $\frac{1}{2}(n+1)(n+2)$ spacetime Killing equations. Thus, $\Delta_aK^a=0$ is a weakening of the familiar spacetime Killing equations. Clearly, if the lapse part of K^a is vanishing and the shift part N^a is tangent to $\mathcal S$ on $\mathcal S$, then $\Delta_aK^a=0$ reduces to the condition $\delta_aN^a=0$ discussed in subsection 2.3.2.

To clarify its compatibility with the evolution equations, let us rewrite the canonical equation of motion for the metric h_{ab} in the spacetime. By (3.17), its right-hand side is just the projection to Σ of the spacetime Killing operator:

$$\dot h_{ab}=2N\chi_{ab}+L_{\mathbf N}h_{ab}=2P^c_aP^d_b\nabla_{(c}K_{d)}.$$

Hence, the contraction of its restriction to $\mathcal S$ with the metric q^{ab} gives $q^{ab}\dot h_{ab}=2\Delta_bK^b$. However, the left-hand side is proportional to the time derivative of the induced volume element on $\mathcal S$: $\dot\varepsilon_{e_1\dots e_{n-1}}=\frac{1}{2}q^{ab}\dot q_{ab}\varepsilon_{e_1\dots e_{n-1}}=\frac{1}{2}q^{ab}\dot h_{ab}\varepsilon_{e_1\dots e_{n-1}}$. Therefore, $\Delta_aK^a=0$ is

precisely the condition that *the induced volume* $(n-1)$*-form on* $\mathcal{S}$ *is constant during the evolution*. Thus the boundary condition $\delta\varepsilon_{e_1\dots e_{n-1}}=0$ for the configuration variables, found in the special cases and discussed in subsections 2.3.1 and 2.3.2, appears naturally in the general case, too.

4.1.5 On Einstein–scalar systems

The quasi-local phase space of the coupled Einstein-scalar system is the cotangent bundle $T^*\mathcal{Q}(\Sigma)$ of the configuration space $\mathcal{Q}(\Sigma)$, the latter being the set of the pairs (h_{ab},Φ), and endowed with the natural symplectic structure. The constraint of the coupled system is $C[N,N^a]:=C_E[N,N^a]+H_S[N,N^a]=0$, where now (1.1) is denoted by $C_E[N,N^a]$ and $H_S[N,N^a]$ is given by (3.5), and the Hamiltonian is the sum of the Hamiltonians of the gravitational and the scalar sectors: $H[N,N^a]=H_E[N,N^a]+H_S[N,N^a]$. However, note that $H_S[N,N^a]$ depends on the metric h_{ab}, which is now a configuration variable. Thus, assuming that both $K^a:=Nt^a+N^a$ and $\bar K^a:=\bar Nt^a+\bar N^a$ are Δ_e–divergence-free, the *formal* Poisson bracket of the Hamiltonians $H[N,N^a]$ and $H[\bar N,\bar N^a]$ is

$$\begin{aligned}\Big\{H\big[N,N^a\big]\,,\,H\big[\bar N,\bar N^a\big]\Big\}=&\\ =C\Big[\bar N^eD_eN-N^eD_e\bar N\,,\,&ND^a\bar N-\bar ND^aN-\big[N,\bar N\big]^a\Big]+\\ +\frac{1}{\kappa}\oint_{\mathcal{S}}\Big\{&\big(\Delta^eK^a\big)\big(\Delta_e\bar K^b\big)\,{}^\perp\varepsilon_{ab}+\lambda\,{}^\perp\varepsilon_{ab}K^a\bar K^a-\\ -\frac{1}{8}&K^a\bar K^bF^{cd}{}_{ef}\,{}^\perp\varepsilon_{gh}\delta^{efgh}_{abcd}+\frac{1}{2}\big(K^a\bar K^b-\bar K^aK^b\big)\,{}^\perp\varepsilon_{ac}\kappa T^c{}_b\Big\}\mathrm{d}\mathcal{S}.\end{aligned}\tag{4.9}$$

Since $F^a{}_{bcd}={}^MR^a{}_{bef}\Pi^e_c\Pi^f_d$, the last three terms of the boundary integral can be written as

$$\begin{aligned}&-\frac{1}{8}K^a\bar K^{b\,M}C^{cd}{}_{ef}\,{}^\perp\varepsilon_{gh}\delta^{efgh}_{abcd}+\\ &+\frac{1}{2}\big(K^a\bar K^b-\bar K^aK^b\big)\,{}^\perp\varepsilon_{ac}\Big({}^MG^c{}_b+\kappa T^c{}_b+\delta^c_b\lambda\Big)+\\ &+\frac{1}{2}\big(K^a\bar K^b-\bar K^aK^b\big)\,{}^\perp\varepsilon_{ac}\Big(\frac{n-3}{n-1}\,{}^MR^c{}_b+\frac{1}{n(n-1)}\,{}^MR\delta^c_b\Big),\end{aligned}$$

where ${}^MC_{abcd}$, ${}^MR_{ab}$ and ${}^MR$ are the spacetime Weyl and Ricci tensors and the curvature scalar, respectively, and the second line is proportional to the expression whose vanishing is just the Einstein equation. Thus, in particular for $n=3$ and 'on shell', the Poisson bracket of two Hamiltonians is the boundary integral of $(\Delta^eK^a)(\Delta_e\bar K^b)\,{}^\perp\varepsilon_{ab}-\frac{1}{2}K^a\bar K^b\,{}^MC_{abcd}\,{}^\perp\varepsilon^{cd}+\frac{1}{6}{}^MRK^a\bar K^b\,{}^\perp\varepsilon_{ab}$. Hence, the trace-free part of the spacetime Ricci tensor does not appear even in the presence of a scalar field.

4.2 Quasi-local quantities from Poisson boundary terms?

In subsection 4.1.2 we raised the idea that the Poisson boundary term should be the sum of the Hamiltonian boundary term (parameterized by the new lapse and shift) and terms analogous to the flux of energy-momentum/angular momentum of matter fields,

and both must be gauge invariant. In the present subsection, we decompose the (gauge-invariant) Poisson boundary term in such a way that the boundary term of the 'improved' basic Hamiltonian (2.13) emerges naturally, even in a (slightly modified) gauge-invariant form. However, as we will see, in its gauge-invariant form it does not seem to yield a representation of the 'composition rule' of how the new lapse and shift are built from the old ones.

We start with (4.5), and let us observe first that in its first line the derivative operator δ_e can be replaced by Δ_e; moreover, the first term in the second line can be written as $\frac{1}{2}(\delta_e\delta^e K^a)\,{}^\perp\varepsilon_{ab}\bar K^b - \frac{1}{2}(\delta_e\delta^e\bar K^a)\,{}^\perp\varepsilon_{ab}K^b$ up to a total δ_e-divergence. Again, by forming total δ_a-divergences, the third line is written as $(\bar K^e\Delta_e K^a - K^e\Delta_e\bar K^b)A_b$ plus extrinsic curvature terms. Thus, for vector fields satisfying $\Delta_a K^a = \Delta_a\bar K^a = 0$, we obtain

$$
\begin{aligned}
\Big\{H\big[N,N^a\big]\,,\,H\big[\bar N,\bar N^a\big]\Big\} &= \qquad\qquad (4.10)\\
&= C\Big[\bar N^e D_e N - N^e D_e\bar N\,,\, ND^a\bar N - \bar N D^a N - \big[N,\bar N\big]^a\Big] - \\
&- \frac{1}{\kappa}\oint_{\mathcal S}\Big\{\big(\bar K^e\Delta_e K_a - K^e\Delta_e\bar K_a\big)\Big({}^\perp\varepsilon^{ab}Q^c{}_{cb} + A^a\Big) + \\
&\quad + \frac{1}{2}\Big(\delta_e\delta^e K^a - 2\big(\delta_c K_d\big)Q^{cda} - 2K^e Q_{cde}Q^{cda} - \\
&\quad - K^c\big(Q_{cfd} - q_{cf}Q^e{}_{ed}\big)A^f\,{}^\perp\varepsilon^{da} + \\
&\quad + \frac{1}{2}K^a\big({}^M R - 2\lambda + \big[Q_{cde} - q_{cd}Q^f{}_{fe}\big]Q^{cde}\big)\Big)\,{}^\perp\varepsilon_{ab}\bar K^b - \\
&\quad - \frac{1}{2}\Big(\delta_e\delta^e\bar K^a - 2\big(\delta_c\bar K_d\big)Q^{cda} - 2\bar K^e Q_{cde}Q^{cda} - \\
&\quad - \bar K^c\big(Q_{cfd} - q_{cf}Q^e{}_{ed}\big)A^f\,{}^\perp\varepsilon^{da} + \\
&\quad + \frac{1}{2}\bar K^a\big({}^M R - 2\lambda + \big[Q_{cde} - q_{cd}Q^f{}_{fe}\big]Q^{cde}\big)\Big)\,{}^\perp\varepsilon_{ab}K^b\Big\}\mathrm{d}\mathcal S.
\end{aligned}
$$

Thus the first line in the boundary integral is just the boundary term of $H_1[K^a]$ given by (2.13), in which K^a is replaced by the 'commutator' $\bar K^e\Delta_e K^a - K^e\Delta_e\bar K^a$. Since, assuming $\Delta_a K^a = \Delta_a\bar K^a = 0$, the integral of (4.5) is invariant with respect to the change of the basis (t^a, v^a) in the normal bundle of $\mathcal S$ ('$SO(1,1)$ boost-gauge invariance'), the decomposition of the integrand of (4.10) to the Hamiltonian boundary term (the first line) and to the rest can be made in a boost-gauge-invariant way, too. In fact, by the Hodge decomposition (see e.g. [30]) the connection 1-form A_e is the sum of an exact, a co-exact and a harmonic 1-form on $\mathcal S$: $A_e = \delta_e\alpha + \alpha_e + \omega_e$, respectively, and this decomposition is unique. Here the function $\alpha:\mathcal S\to\mathbb R$ is unique up to an additive constant, α_e is δ_e-divergence free, while ω_e is both δ_e-divergence free and satisfies $\delta_{[a}\omega_{b]} = 0$. (The first represents the pure gauge part of A_e, the co-exact part yields curvature, and the harmonic part only holonomy, but no curvature.) Thus by $\delta_{[a}A_{b]} = \delta_{[a}\alpha_{b]}$ it is only the co-exact part of A_e that appears in (4.5), and hence we can substitute A_e by α_e in (4.10), too, yielding a manifestly boost gauge invariant form of the 'improved' basic Hamiltonian. Another interpretation of the above Hodge decomposition is that it provides a 'natural' gauge fixing, using only the intrinsic geometry of $\mathcal S$.

Unfortunately, however, this Hamiltonian boundary term does not seem to represent the 'composition rule' of the lapses and shifts in a correct way. Indeed, the lapse-shift parts of $\bar K^e\Delta_e K^a - K^e\Delta_e\bar K^a$ are *not* the new lapse $\bar N^e D_e N - N^e D_e\bar N$ and the new shift $ND^a\bar N - \bar N D^a N - [N,\bar N]^a$ that appear in the constraint function.

5 Conclusions

We learnt from the quasi-local canonical formulation of the scalar field that the Poisson boundary terms represent energy-momentum and angular momentum fluxes out from and into the localized system, i.e. they are well defined physical quantities. Here we raise the idea that the same may be expected in general relativity, too, and hence the Poisson boundary term in GR must be gauge invariant in every sense. We showed that this requirement yields the condition for the lapse and shift that the spacetime vector field that they determine must be divergence free with respect to a Sen-type connection on the boundary. This condition is a part of the spacetime Killing equations. This yields that the evolution equations preserve the volume form induced on the boundary. Therefore, keeping the induced volume form fixed as a condition seems to be the part of the (yet unknown) 'ultimate' boundary conditions for the canonical variables. This implies that the quasi-local constraint algebra that we found earlier (and discussed in subsection 2.3.1) is probably the 'correct' one, completing the point (iii) of subsection 2.1.1.

We also found arguments both in favour of and against the Hamiltonian boundary term in $H_1[K^a]$. It appears naturally as a part of the Poisson boundary term and its $SO(1,1)$ boost-gauge dependence can be cured, but, without additional restrictions on the lapse and the shift it does not yield functionally differentiable Hamiltonian, and it does not represent the composition law for the lapses and shifts in a correct way.

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